



UNIVERSIDADE ESTADUAL PAULISTA “JÚLIO DE MESQUITA FILHO”

PROGRAMA DE PÓS-GRADUAÇÃO EM CIÊNCIAS DOS MATERIAIS

Departamento de Física e química - DFQ

Propriedades espectrais de férmions de Majorana na presença da interação de Ising

Luana Teodoro Lustosa

Ilha Solteira - SP

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Orientador: Prof. Dr. Antonio Carlos Ferreira Seridonio

Dissertação apresentada à Universidade Estadual Paulista "Júlio Mesquita Filho" Unesp - Faculdade de Engenharia de Ilha Solteira, para obtenção do título de mestre em Ciências dos Materiais.

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Ilha Solteira, 28 de fevereiro de 2024

Em memória de meu avô José Teodoro.

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*“Somente aqueles que sofreram por
muito tempo conseguem ver luz através
das sombras”*

*“O mais bravo não é aquele que ganha,
mas sim aquele que encara seus medos”.*

Roronoa Zoro

Resumo

Investigamos as propriedades espectrais de uma impureza quântica (QI - quantum impurity) de forma teórica e encontramos, o que propomos chamar de excitação de quasipartícula do tipo Majorana-Ising (MIQ - Majorana-Ising quasiparticle). Essa, surge do acoplamento entre um supercondutor topológico (TSC - topological superconductor) finito baseado em uma cadeia supercondutora de átomos magnéticos e um spin S inteiro que flanqueia a QI. Esse spin S acopla-se a impureza pela interação de troca do tipo Ising. Como os modos zero de Majorana (MZMs - Majorana zero-modes) estão superpostos nas bordas da cadeia supercondutora, contra intuitivamente, encontramos um regime em que o termo de Ising modula a localização da ressonância do MZM fracionalizado no sítio da impureza. A natureza fermiônica desse estado é revelada como puramente eletrônica e com uma condutância de Andreev completamente nula em sua origem. Portanto, descobrimos um estado de borda ressonante como um modo zero no sistema.

Palavras-chave: Férmions de Majorana, fio de Kitaev, impureza quântica.

Abstract

We theoretically investigate the spectral properties of a quantum impurity (QI) hosting the here proposed Majorana-Ising-type quasiparticle (MIQ) excitation. It arises from the coupling between a finite topological superconductor (TSC) based on a chain of magnetic adatoms-superconducting hybrid system and an integer large spin S flanking the QI. Noteworthy, the spin S couples to the QI via the Ising-type exchange interaction. As the Majorana zero-modes (MZMs) at the edges of the TSC chain are overlapped, we find a regime wherein the Ising term modulates the localization of a fractionalized and resonant MZM at the QI site. Therefore, the fermionic nature of this state is revealed as purely of electron tunneling-type and has the Andreev conductance completely null in its birth. As a result, we find that a resonant edge state appears as a zero-mode in the system.

Keywords: Majorana fermions, Kitaev wire, quantum impurity.

Sumário

1	Introdução	10
2	Formalismo matemático	13
2.1	Fio de Kitaev (toy model)	13
2.2	Propriedades de Bulk	16
2.3	Modelo de Anderson para uma impureza	24
2.4	Funções de Green	25
2.5	Equação de movimento	26
3	Modelo teórico	29
3.1	Hamiltoniano do sistema	29
3.2	Desenvolvimento das funções de Green	34
3.3	Impureza quântica escrita na base de férmions de Majorana	38
4	Resultados e Discussão	41
4.1	Quasipartícula do tipo Majorana-Ising	41
4.1.1	Condutância	41
4.1.2	Excitação de quasipartícula do tipo Majorana-Ising e seus perfis espectrais	43
5	Conclusões	50
6	Publicações e perspectivas futuras	51
7	Impacto e relevância científico-social	52
A	Apêndice	58
A.1	Obtenção das funções de Green	58
A.1.1	Funções de Green encontradas	86

A.1.2 Para o Spin-up	87
A.2 Artigo publicado	92

Capítulo 1

Introdução

O físico italiano Ettore Majorana propôs há quase um século, no contexto da Física de altas energias, a existência de férmions que possuem sua partícula igual a sua própria antipartícula, descritas pela solução real da equação de Dirac [1], conhecidos como férmions de Majorana. Na Física da Matéria Condensada, esses férmions surgem como excitações de quasipartículas. Dentro desse âmbito, duas quasipartículas de Majorana separadas podem definir um único férmion regular não local. Essa propriedade intrigante possibilita a utilização desses férmions específicos na construção de um quantum bit (qubit) protegido, ou seja, livre de influências externas e imune a fenômenos de decoerência quântica. O qubit é fundamental no avanço da computação quântica, e, por essa razão, pesquisadores na área de informação quântica têm concentrado esforços na busca por dispositivos baseados em férmions de Majorana

Essas excitações de quasipartícula são usualmente denotadas como modos zero de Majorana (MZMs - no inglês, Majorana zero-modes), que são encontrados nas bordas de um supercondutor topológico (TSC - Topological superconductor) [2–31]. Desde a proposta teórica feita por Kitaev [32], MZMs são cobigados por suas características e possível aplicação na computação quântica topológica livre de falhas.

Previsões teóricas apontam que há um pico fracionalizado de condutância com energia zero na análise de transporte eletrônico através de pontos quânticos, que é dado por $\mathcal{G}_{\text{Total}}(0) = \frac{e^2}{2h}$ [2–4]. Esse, por sua vez, pode ter origem no regime trivial, podendo exibir estados ligados de Andreev (ABS - Andreev bound states) [29, 33].

No regime não-trivial, dois MZMs emergem espacialmente separados nas bordas do TSC. Um férmion regular pode ser decomposto em dois MZMs, que apresentam, individualmente, uma amplitude na condutância de $\mathcal{G}_{\text{Total}}(0) = \frac{e^2}{2h}$, o que evidencia a fracionalização do *quantum*

de condutância, dando origem ao conceito de elétron fracionalizado e revelando a natureza de “meio férmion” do MZM [4]. Esse tipo de assinatura emerge em plataformas que combinam supercondutividade do tipo “s”, forte acoplamento spin-orbita (SOC- spin-orbit coupling) e campo magnético. Como resultado, torna-se possível a supercondutividade do tipo “p”, que foi induzida no sistema por efeito de proximidade, permitindo a realização experimental do fio de Kitaev *spinless*, que representa um TSC em uma dimensão. Para a produção do fio de Kitaev, destacam-se duas formas para sua realização experimental: (i) um nanofio semicondutor com SOC que deve ser depositado sobre um supercondutor do tipo “s”, na presença de um campo magnético, ou (ii) uma cadeia linear de átomos magnéticos com interações de troca, hospedada por um supercondutor do tipo “s” com forte SOC. Nessas situações, o supercondutor do tipo “s” com par de Cooper singlete induz à supercondutividade por efeito de proximidade, que é fundamental para gerar o caráter supercondutor (SC - superconducting), nos fios de Kitaev produzidos. Então, o campo Zeeman e o SOC de tais materiais quânticos induzem a SC do tipo “p” no sistema. Emergindo então, o par de Cooper tripleto, que é o responsável pela supercondutividade do tipo “p”.

Particularmente, no regime topológico não trivial dessas configurações, essas excitações de quasipartículas de Majorana emergem de maneira ideal, ou seja, como MZMs desacoplados entre si e localizados nas bordas do TSC. Devido a esse desacoplamento, os MZMs são considerados robustos contra perturbações, uma vez que são protegidos topologicamente pelo *gap* do SC. Assim, os MZMs tornam-se candidatos promissores para a computação quântica livre do fenômeno da decoerência [34, 35]. No entanto, MZMs perfeitamente desacoplados uns dos outros são objetos hipotéticos, uma vez que eles são observados apenas em sistemas de tamanho infinito e, em experimentos reais, os fios quânticos são finitos. Como resultado, esses MZMs presentes nas bordas de um fio finito superpõem-se e, inevitavelmente, um modo fermiônico com uma energia finita emerge.

Para transpassar esse desafio, neste trabalho, encontramos uma forma de fracionalizar um MZM, em particular, aquele encontrado no sítio da impureza quântica (QI - quantum impurity) acoplada a uma das bordas do TSC finito em uma dimensão. Para isso, devemos levar em consideração a interação de troca de Ising entre um spin inteiro e a impureza. Esse sistema corresponde à situação em que os MZMs γ_1 e γ_2 estão localizados nas bordas de um TSC finito. Esses objetos, que podem ser representados como semi-esferas, ilustram o MZM e explica diagramaticamente o elétron fracionalizado que obtivemos, assim como o MZM também

fracionalizado.

Essas semi-esferas compõem a esfera inteira delocalizada, onde cada semi-esfera está disposta nas extremidade do TSC, emulando a natureza não-local do estado fermiônico composto pelos MZMs, que estão espacialmente separados. O peso espectral de Majorana, em particular para a QI acoplada ao TSC finito, é dado pelo valor unitário quando há o vazamento do MZM γ_1 para dentro do ponto quântico [4]. Essa unidade corresponde a semi-esfera, que representa o estado de meio elétron que contribui com $\mathcal{G}_{\text{Total}}(0) = \frac{e^2}{2h}$, como esperado.

Particularmente para um TSC finito, definimos um ponto especial do sistema que possui uma configuração específica, em que a interação de troca de Ising permite que seja observado um MZM fracionalizado γ_{MIQ} na QI, que chamamos de excitação de quasipartícula do tipo Majorana-Ising (MIQ - Majorana-Ising quasiparticle). Simbolizando um novo tipo de excitação de MZM na presença de TSC finito, identificado por um peso espectral de Majorana igual a metade, correspondendo a $\frac{1}{4}$ do sítio eletrônico da QI, apresentando $\mathcal{G}_{\gamma_{MIQ}}(0) = \frac{e^2}{4h}$.

Apenas para umas das DOSs (density of states - densidade de estados) de Majorana no sítio da QI o MIQ emerge como estado ressonante localizado em $\omega = 0$. O outro MZM de Majorana da QI apresenta um estado antirressonante, mas apresenta a mesma amplitude do estado ressonante de um férmion de Majorana. Dessa maneira, podemos afirmar que um novo tipo de MZM é encontrado no sítio da QI. Nessa situação, demonstramos que a emergência de tal tipo de quasipartícula produz a condutância de Andreev completamente nula na voltagem zero, na qual existe apenas a contribuição eletrônica para a condutância total.

Desse modo, este trabalho foi dividido para uma melhor apresentação dos resultados encontrados, da seguinte forma: no capítulo 2 será apresentado o formalismo matemático utilizado para a resolução analítica do problema, composto pelo fio de Kitaev (toy model) e suas propriedades de bulk, modelo de Anderson, funções de Green e equação de movimento. Já no capítulo 3 será apresentado o modelo teórico estudado para a obtenção do resultado deste trabalho. No capítulo 4 serão apresentados os resultados e discussões sobre a excitação de quasipartícula do tipo Majorana-Ising, MIQ. O capítulo 5 apresentará as conclusões sobre este trabalho, em que foi possível observar a fracionalização de um férmion de Majorana, a MIQ. No capítulo 6 serão apresentadas as publicações e perspectivas futuras. No capítulo 7 aparecerá a relevância científico-social deste trabalho. E, por fim, serão apresentados os apêndices que contém o desenvolvimento analítico feito para a realização deste trabalho e o artigo que publicamos [PHYSICAL REVIEW B 107, 155144 (2023)].

Capítulo 2

Formalismo matemático

Este capítulo tem por objetivo apresentar formalismo matemático utilizado para o desenvolvimento deste trabalho, como: o toy model para o fio de Kitaev e suas propriedades de bulk, modelo Modelo de Anderson para uma impureza, funções de Green e equação de movimento (EOM - equation of motion).

2.1 Fio de Kitaev (toy model)

O fio de Kitaev emerge como um candidato altamente promissor para a concretização de Modos zero de Majorana (MZMs), conforme previamente abordado. A concepção desse modelo data de 2001 e foi proposto pelo físico russo Alexei Kitaev, que na época estava envolvido em iniciativas de computação quântica para a Microsoft [32]. Nesse modelo teórico, um nanofio unidimensional desprovido de spin e exibindo supercondutividade do tipo "p", apresenta-se como uma rede tight-binding e é descrito pelo Hamiltoniano a seguir [25, 32].

$$H = -\mu \sum_x c_x^\dagger c_x - \frac{1}{2} \sum_x (t c_x^\dagger c_{x+1} + \Delta e^{i\phi} c_x c_{x+1} + \text{H.c.}), \quad (2.1)$$

em que μ é o potencial químico, t descreve o hopping entre primeiros vizinhos e Δ representa a amplitude de ligação do par de Cooper para supercondutividade do tipo "p", com fase ϕ correspondente.

Os operadores fermiônicos c_x podem ser escritos em termos de dois férmions de Majorana,

$$c_x = \frac{e^{-i\phi/2}}{2} (\gamma_{B,x} + i\gamma_{A,x}) \quad (2.2)$$

e

$$c_x^\dagger = \frac{e^{i\phi/2}}{2}(\gamma_{B,x} - i\gamma_{A,x}). \quad (2.3)$$

Tais operadores obedecem as relações $\{\gamma_{\alpha,x}, \gamma_{\alpha',x'}\} = 2\delta_{\alpha\alpha'}\delta_{xx'}$, o que leva à $\gamma_{\alpha,x}^2 = 1$.

Substituindo as Eq. (2.2) e (2.3) na Eq. (2.1), temos

$$\begin{aligned} \mathcal{H} = & -\frac{\mu}{4} \sum_x (\gamma_{B,x}\gamma_{B,x} + i\gamma_{B,x}\gamma_{A,x} - i\gamma_{A,x}\gamma_{B,x} + \gamma_{A,x}\gamma_{A,x}) \\ & - \frac{t}{8} \sum_x (\gamma_{B,x}\gamma_{B,x+1} + i\gamma_{B,x}\gamma_{A,x+1} - i\gamma_{A,x}\gamma_{B,x+1} + \gamma_{A,x}\gamma_{A,x+1}) \\ & + \frac{t}{8} \sum_x (\gamma_{B,x}\gamma_{B,x+1} + i\gamma_{A,x}\gamma_{B,x+1} - i\gamma_{B,x}\gamma_{A,x+1} + \gamma_{A,x}\gamma_{A,x+1}) \\ & - \frac{\Delta}{8} \sum_x (\gamma_{B,x}\gamma_{B,x+1} + i\gamma_{B,x}\gamma_{A,x+1} + i\gamma_{A,x}\gamma_{B,x+1} - \gamma_{A,x}\gamma_{A,x+1}) \\ & + \frac{\Delta}{8} \sum_x (\gamma_{B,x}\gamma_{B,x+1} - i\gamma_{B,x}\gamma_{A,x+1} - i\gamma_{A,x}\gamma_{B,x+1} - \gamma_{A,x}\gamma_{A,x+1}), \end{aligned} \quad (2.4)$$

simplificando, temos

$$\begin{aligned} \mathcal{H} = & -\frac{\mu}{4} \sum_x (\gamma_{B,x}\gamma_{B,x} + i\gamma_{B,x}\gamma_{A,x} - i\gamma_{A,x}\gamma_{B,x} + \gamma_{A,x}\gamma_{A,x}) \\ & - \frac{it}{4} \sum_x (\gamma_{B,x}\gamma_{A,x+1} - \gamma_{A,x}\gamma_{B,x+1}) \\ & - \frac{i\Delta}{4} \sum_x (\gamma_{B,x}\gamma_{A,x+1} + \gamma_{A,x}\gamma_{B,x+1}). \end{aligned} \quad (2.5)$$

Utilizando a relação $\{\gamma_{A,x}, \gamma_{B,x}\} = 0$ e $\gamma_{a,x}^2 = 1$, obtém-se

$$\begin{aligned} \mathcal{H} = & -\frac{\mu}{4} \sum_x (\gamma_{B,x}\gamma_{B,x} + \gamma_{A,x}\gamma_{A,x}) \\ & - \frac{it}{4} \sum_x (\gamma_{B,x}\gamma_{A,x+1} - \gamma_{A,x}\gamma_{B,x+1}) \\ & - \frac{i\Delta}{4} \sum_x (\gamma_{B,x}\gamma_{A,x+1} + \gamma_{A,x}\gamma_{B,x+1}), \end{aligned} \quad (2.6)$$

então,

$$\mathcal{H} = -\frac{\mu}{2} \sum_{x=1}^N (1 + i\gamma_{B,x}\gamma_{A,x}) - \frac{i}{4} \sum_{x=1}^{N-1} (t + \Delta)\gamma_{B,x}\gamma_{A,x+1} - \frac{i}{4} \sum_{x=1}^{N-1} (t - \Delta)\gamma_{A,x}\gamma_{B,x+1} \quad (2.7)$$

Na abordagem proposta por Kitaev, são considerados dois casos limites. O primeiro é denominado como a fase trivial, que se manifesta quando $\mu \neq 0$ e $t = \Delta = 0$. Nessa condição, o Hamiltoniano da Eq. (2.7) simplifica-se para conter apenas o primeiro termo, ou seja

$$\mathcal{H} = -\frac{\mu}{2} \sum_{x=1}^N (1 + i\gamma_{B,x}\gamma_{A,x}), \quad (2.8)$$

que representa a ligação entre Majoranas de mesmo sítio e não há nenhum acoplamento entre Majoranas de sítios vizinhos, como pode ser visto na Fig. 2.1.

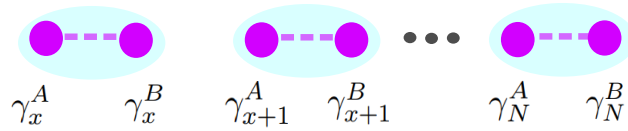


Figura 2.1: Ilustração do fio de Kitaev na chamada fase trivial. As elipses em ciano representam os sítios da rede e os círculos roxos representam os férmions de Majoranas acoplados que compõem esse mesmo sítio.

O segundo caso limite, chamado de fase topológica, obedece as condições $\mu = 0$ e $t = \Delta \neq 0$. Dessa forma, o Hamiltoniano da Eq. (2.7) simplifica-se para conter apenas o termo,

$$\mathcal{H} = -i\frac{t}{2} \sum_{x=1}^{N-1} \gamma_{B,x}\gamma_{A,x+1}, \quad (2.9)$$

na configuração específica apresentada, apenas os férmions de Majorana nos sítios adjacentes da rede estão acoplados. Essa disposição resulta no desacoplamento dos estados de Majorana $\gamma_{A,1}$ e $\gamma_{B,N}$ localizados nas extremidades da cadeia, (2.2). Esses Majoranas isolados emergem como promissores candidatos para o qubit quântico, estando desacoplados do resto do sistema prevenindo a perda de informações devido a fenômenos de decoerência quântica.

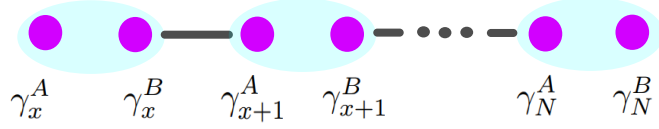


Figura 2.2: Ilustração do fio de Kitaev na fase topológica, onde só há acoplamento entre Majoranas de sítios adjacentes da rede, fazendo com que emerge nas extremidades da cadeia os MZMs (modo zero de Majorana - Majorana zero mode) isolados.

Desta forma, os dois férmions de Majorana isolados nas bordas do sistema, podem ser reescritos dando origem a um estado fermiônico descrito como,

$$f = \frac{1}{2}(\gamma_{A,1} + i\gamma_{B,N}) \quad (2.10)$$

O operador fermiônico f é considerado não local, uma vez que os MZMs que o compõem estão espacialmente separados Fig. 2.3.

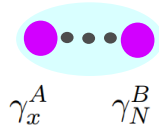


Figura 2.3: Ilustração do formação do férmion não-local composto pelos MZMs que se encontram isolados nas bordas da cadeia.

2.2 Propriedades de Bulk

Para investigar as propriedades de bulk no modelo Kitaev é essencial analisar o sistema no espaço de momento k dentro de condições periódica de contorno [2, 25, 36, 37]. Neste contexto, começamos reescrevendo os operadores de sítio do Hamiltoniano original (Eq. 2.1) no espaço de momento, considerando uma série de Fourier da seguinte maneira [38],

$$c_x = \frac{1}{\sqrt{N}} \sum_k e^{-ikxa} c_k \quad (2.11)$$

e

$$c_x^\dagger = \frac{1}{\sqrt{N}} \sum_k e^{-ikxa} c_k^\dagger \quad (2.12)$$

sendo a o parâmetro de rede. De acordo com essa definição,

$$\begin{aligned} \sum_{x=1}^N c_x^\dagger c_x &= \sum_{x=1}^N \frac{1}{\sqrt{N}} \sum_k e^{ikxa} c_k^\dagger \frac{1}{\sqrt{N}} \sum_{k'} e^{-ik'xa} c_{k'}' \\ &= \sum_{x=1}^N \frac{1}{N} \sum_{kk'} e^{i(k-k')xa} c_k^\dagger c_{k'}' \\ &= \sum_{kk'} c_k^\dagger c_{k'}' \sum_{x=1}^N \frac{1}{N} e^{i(k-k')xa} \\ &= \sum_{kk'} c_k^\dagger c_{k'}' \delta_{kk'} \\ &= \sum_k c_k^\dagger c_k \end{aligned} \quad (2.13)$$

A definição de delta de Kronecker é:

$$\delta_{kk'} = \sum_{x=1}^N \frac{1}{N} e^{i(k-k')xa} = \begin{cases} 0, & \text{se } k \neq k' \\ 1, & \text{se } k = k' \end{cases}. \quad (2.14)$$

Da mesma forma,

$$\begin{aligned}
\sum_{x=1}^{N-1} c_x^\dagger c_{x+1} &= \sum_{x=1}^{N-1} \frac{1}{\sqrt{N}} \sum_k e^{ikxa} c_k^\dagger \frac{1}{\sqrt{N}} \sum_{k'} e^{-ik'(x+1)a} c_{k'} \\
&= \sum_{x=1}^{N-1} \frac{1}{N} \sum_{kk'} e^{ikxa} e^{-ik'(x+1)a} c_k^\dagger c_{k'} \\
&= \sum_{kk'} e^{-ik'a} c_k^\dagger c_{k'} \sum_{x=1}^{N-1} \frac{1}{N} e^{i(k-k')xa} \\
&= \sum_{kk'} e^{-ik'a} c_k^\dagger c_{k'} \delta_{kk'} \\
&= \sum_k e^{-ika} c_k^\dagger c_k,
\end{aligned} \tag{2.15}$$

$$\begin{aligned}
\sum_{x=1}^{N-1} c_{x+1}^\dagger c_x &= \sum_{x=1}^{N-1} \frac{1}{\sqrt{N}} \sum_k e^{ik(x+1)a} c_k^\dagger \frac{1}{\sqrt{N}} \sum_{k'} e^{-ik'xa} c_{k'} \\
&= \sum_{x=1}^{N-1} \frac{1}{N} \sum_{kk'} e^{ik(x+1)a} e^{-ik'xa} c_x c_{k'} \\
&= \sum_{kk'} e^{ika} c_x c_{k'} \sum_{x=1}^{N-1} \frac{1}{N} e^{i(k-k')xa} \\
&= \sum_{kk'} e^{ika} c_x c_{k'} \delta_{kk'} \\
&= \sum_{kk'} e^{ika} c_x c_{k'},
\end{aligned} \tag{2.16}$$

e

$$\begin{aligned}
\sum_{x=1}^{N-1} c_x c_{x+1} &= \sum_{x=1}^{N-1} \frac{1}{\sqrt{N}} \sum_k e^{-ikxa} c_k \frac{1}{\sqrt{N}} \sum_{k'} e^{-ik'(x+1)a} c_{k'} \\
&= \sum_{x=1}^{N-1} \frac{1}{N} \sum_{kk'} e^{-ikxa} e^{-ik'xa} e^{-ik'a} c_k c_{k'} \\
&= \sum_{kk'} e^{-ik'a} c_k c_{k'} \sum_{x=1}^{N-1} \frac{1}{N} e^{-i(k+k')xa} \\
&= \sum_{kk'} e^{-ik'a} c_k c_{k'} \delta_{k,-k'} \\
&= \sum_k e^{-ik'a} c_k c_{-k} \\
&= \sum_k e^{-ika} c_{-k} c_k
\end{aligned} \tag{2.17}$$

O Hermitiano conjugado é obtido de forma análoga,

$$\sum_{x=1}^{N-1} c_x^\dagger c_{x+1}^\dagger = \sum_k e^{ika} c_{-k}^\dagger c_{-k}^\dagger \tag{2.18}$$

Então, o Hamiltoniano no espaço dos momentos, fica,

$$\mathcal{H} = -\mu \sum_k c_k^\dagger c_k - \frac{1}{2} \sum_k t (e^{-ika} c_k^\dagger c_k^\dagger + e^{ika} c_k^\dagger c_k^\dagger) \tag{2.19}$$

$$\begin{aligned}
&- \frac{1}{2} \sum_k \Delta (e^{-ika} c_{-k} c_k + e^{ika} c_k^\dagger c_{-k}^\dagger) \\
&= \sum_k (-\mu - t \cos(ka)) c_k^\dagger c_k - \frac{\Delta}{2} \sum_k (e^{-ika} c_{-k} c_k + e^{ika} c_k^\dagger c_{-k}^\dagger) \\
&= \sum_k \varepsilon_k c_k^\dagger c_k - \frac{\Delta}{2} \sum_k ((e^{-ika} c_{-k} c_k) + e^{ika} c_k^\dagger c_{-k}^\dagger)
\end{aligned} \tag{2.20}$$

Com $\varepsilon_k = -\mu - t \cos(ka)$ sendo a energia cinética. O hamiltoniano pode ser reescrito de forma mais compacta,

$$\begin{aligned}
\sum_k \varepsilon_k c_k^\dagger c_k &= \frac{1}{2} \sum_k (\varepsilon_k c_k^\dagger c_k + \varepsilon_k c_k^\dagger c_k) \\
&= \frac{1}{2} \sum_k (\varepsilon_k c_k^\dagger c_k + \varepsilon_k (1 - c_k c_k^\dagger)) \\
&= \frac{1}{2} \sum_k (\varepsilon_k c_k^\dagger c_k - \varepsilon_{-k} c_{-k} c_{-k}^\dagger) + \frac{1}{2} \sum_k \varepsilon_k,
\end{aligned} \tag{2.21}$$

$$\begin{aligned}
\sum_k e^{-ika} c_{-k} c_k &= \frac{1}{2} \sum_k (e^{-ika} c_{-k} c_k + e^{-ika} c_{-k} c_k) \\
&= \frac{1}{2} \sum_k (e^{-ika} c_{-k} c_k - e^{-ika} c_k c_{-k}) \\
&= \frac{1}{2} \sum_k (e^{-ika} c_{-k} c_k - e^{ika} c_{-k} c_k) \\
&= \frac{1}{2} \sum_k c_{-k} c_k (e^{-ika} - e^{ika}) \\
&= - \sum_k i \sin(ka) c_{-k} c_k
\end{aligned} \tag{2.22}$$

e

$$\begin{aligned}
\sum_k e^{ika} c_k^\dagger c_{-k}^\dagger &= \frac{1}{2} \sum_k (e^{ika} c_k^\dagger c_{-k}^\dagger + e^{ika} c_k^\dagger c_{-k}^\dagger) \\
&= \frac{1}{2} \sum_k (e^{ika} c_k^\dagger c_{-k}^\dagger - e^{ika} c_{-k}^\dagger c_k^\dagger) \\
&= \frac{1}{2} \sum_k (e^{ika} c_k^\dagger c_{-k}^\dagger - e^{-ika} c_k^\dagger c_{-k}^\dagger) \\
&= \sum_k i \sin(ka) c_k^\dagger c_{-k}^\dagger.
\end{aligned} \tag{2.23}$$

Desta forma,

$$\begin{aligned}
\mathcal{H} &= \frac{1}{2} \sum_k (\varepsilon_k c_k^\dagger c_k - \varepsilon_{-k} c_{-k} c_{-k}^\dagger) - \frac{\Delta}{2} \sum_k i \sin(ka) c_{-k} c_k + \frac{\Delta}{2} \sum_k i \sin(ka) c_k^\dagger c_{-k}^\dagger + \frac{1}{2} \sum_k \varepsilon_k \\
&= \frac{1}{2} \sum_k (\varepsilon_k c_k^\dagger c_k - \varepsilon_{-k} c_{-k} c_{-k}^\dagger + \frac{1}{2} \sum_k \Delta_k c_{-k} c_k + \frac{1}{2} \sum_k \Delta_k^* c_k^\dagger c_{-k}^\dagger) + \frac{1}{2} \sum_k \varepsilon_k \\
&= \frac{1}{2} \sum_k (\varepsilon_k c_k^\dagger c_k - \varepsilon_{-k} c_{-k} c_{-k}^\dagger + \Delta c_{-k} c_k + \Delta^* c_k^\dagger c_{-k}^\dagger) + \frac{1}{2} \sum_k \varepsilon_k,
\end{aligned} \tag{2.24}$$

$\Delta_k = -i \sin(ka)$ descreve a energia de emparelhamento supercondutora da transformada de Fourier. Podemos reescrever a Eq. (2.24) em uma representação equivalente de matriz (omitindo a constante),

$$\mathcal{H} = \frac{1}{2} \sum_k (c_{y_k} c_{-k}) \begin{pmatrix} \varepsilon_k & \Delta_k^* \\ \Delta_k & -\varepsilon_{-k} \end{pmatrix} \begin{pmatrix} c_k \\ c_{-k}^\dagger \end{pmatrix}. \tag{2.25}$$

É comum definirmos os espinores de Nambu, em sistemas supercondutores [38] como,

$$\Psi_k^\dagger = \begin{pmatrix} c_k^\dagger & c_{-k}^\dagger \end{pmatrix} \tag{2.26}$$

e

$$\Psi_k = \begin{pmatrix} c_k \\ c_{-k}^\dagger \end{pmatrix} \tag{2.27}$$

E, finalmente

$$\mathcal{H} = \frac{1}{2} \sum_k \Psi_k^\dagger \mathcal{H}_{BdG} \Psi_k \tag{2.28}$$

Sendo o Hamiltoniano de BdG,

$$\mathcal{H}_{BdG} = \begin{pmatrix} \varepsilon_k & \Delta_k^* \\ \Delta_k & -\varepsilon_{-k} \end{pmatrix}. \quad (2.29)$$

Os níveis de energia E_k são dados pela equação a seguir:

$$|\mathcal{H}_{BdG} - E(k)I| = 0, \quad (2.30)$$

em que $E(k)$ são as autoenergias associadas ao $\mathcal{H}_{BdG}$ e I é a matriz identidade 2×2 . A solução da expressão gera duas bandas de dispersão [2]

$$E(k)_\pm = \pm \sqrt{\varepsilon_k^2 + |\Delta_k|^2} = \pm \sqrt{(\mu + t \cos(ka))^2 + \Delta^2 \sin^2(ka)}. \quad (2.31)$$

A Figura 2.4 mostra a dispersão de energia E_k para as quasipartículas supercondutoras (linhas laranja contínuas) e para os elétrons normais (linhas verde tracejadas), para diferentes valores do potencial químico μ . O sistema exibe um "gap" de energia quando $|\mu| > t$ (painéis a) e f)), indicando a presença de supercondutividade. De acordo com a Eq. (2.31), o "gap" fecha quando $|\Delta_k| = \Delta \sin(ka) = 0$ e quando $\varepsilon_k = -\mu - t \cos(ka) = 0$, em que ε_k é a energia cinética dos elétrons. Isso ocorre para $k = 0$ e $k = \pm\pi$, além de $k = k_F$, onde k_F é o momento de Fermi. O fechamento do "gap" de energia ocorre quando $\mu = \pm t$ (painéis b) e d)), indicando a transição entre regimes de emparelhamento forte e fraco. Esta transição é crucial para as propriedades topológicas do sistema, incluindo a emergência de modos de energia zero conhecidos como Majorana bound states (MBSs) no regime de emparelhamento fraco [2, 25, 36]. Os painéis c) e d) representam a condição $|\mu| < t$ em que, nesse intervalo, a dispersão eletrônica ε_k não apresenta um gap, caracterizando o comportamento metálico. Já a dispersão das quasipartículas supercondutoras E_k é definida por um gap finito.

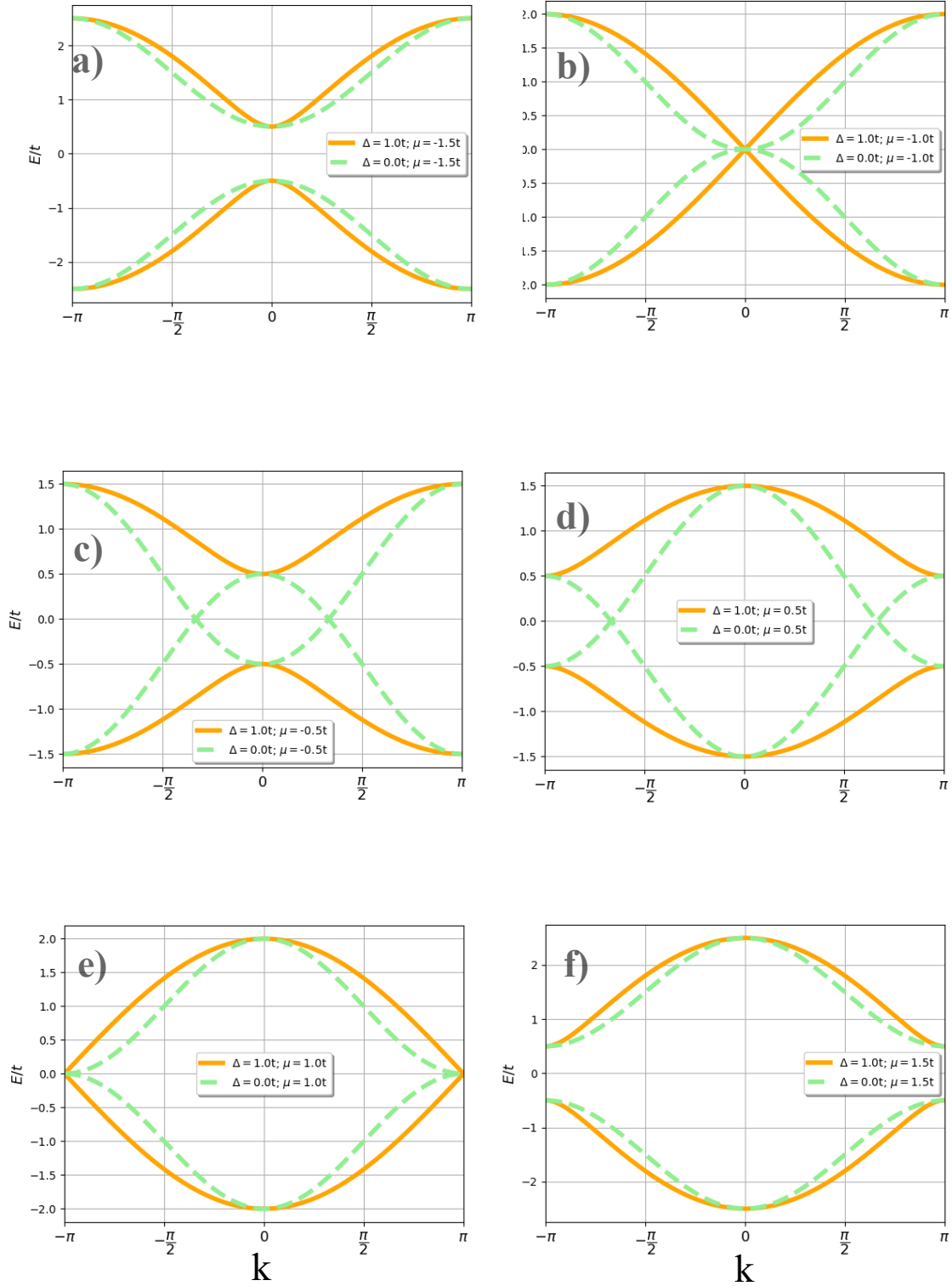


Figura 2.4: A energia das quasipartículas supercondutoras E_k , representada pelas linhas contínuas laranja com $\Delta = t/2$, e a energia dos elétrons na ausência da influência supercondutora ϵ_k , mostrada pelas linhas verde tracejadas com $\Delta = 0$, foram calculadas a partir da Eq. (2.31) do modelo de Kitaev, considerando diferentes valores de potencial químico μ . Observa-se que E_k e ϵ_k apresentam um *gap* quando $\mu < -t$ (painel a) e também quando $\mu > t$ (painel f). Este *gap* se fecha nos pontos $k = 0$ quando $\mu = -t$ e $k = \pm\pi$ quando $\mu = t$, conforme ilustrado nos painéis (b) e (e), respectivamente. No entanto, quando $|\mu| < t$, a dispersão para ϵ_k exibe um caráter metálico, enquanto ocorre a reabertura do *gap* para a dispersão E_k .

2.3 Modelo de Anderson para uma impureza

O modelo de Anderson de uma impureza (SIAM - single impurity Anderson model) foi proposto por P. W. Anderson em 1961 e estuda a correlação de muitos corpos de uma impureza magnética com uma matriz não magnética [39, 40]

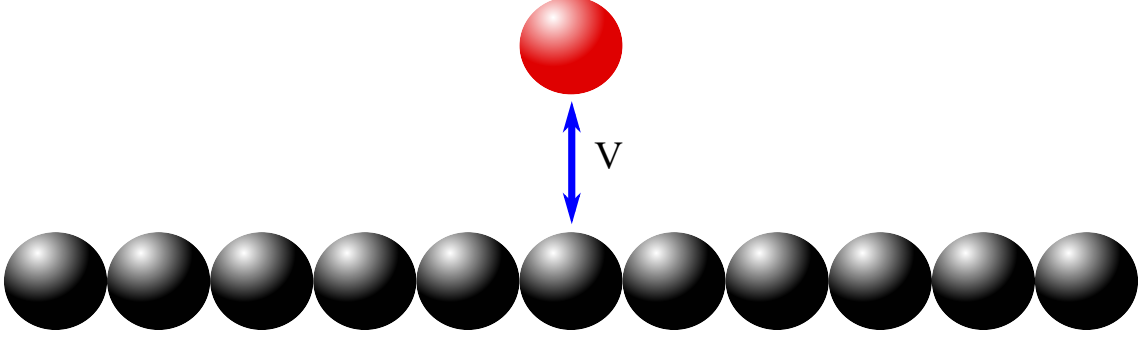


Figura 2.5: Modelo de Anderson com uma impureza magnética (esfera vermelha) sobre uma matriz metálica não magnética, V é a amplitude de hibridização entre impureza e hospedeiro metálico.

A Fig. 2.5 representa um sistema em que o SIAM está presente, este sistema é composto por uma impureza e uma matriz hospedeira e procura estudar a interação entre a impureza e o hospedeiro. O Hamiltoniano de Anderson que expressa a energia deste sistema é dado por

$$\mathcal{H}_{SIAM} = \mathcal{H}_{host} + \mathcal{H}_{imp} + \mathcal{H}_{hib}. \quad (2.32)$$

O primeiro termo do Hamiltoniano da Eq. (2.32) descreve o hospedeiro (gás de elétrons):

$$\mathcal{H}_{host} = \sum_{\sigma \mathbf{k}} \varepsilon_{\mathbf{k}} c_{\sigma \mathbf{k}}^{\dagger} c_{\sigma \mathbf{k}}, \quad (2.33)$$

onde $\varepsilon_{\mathbf{k}}$ descreve a energia dos elétrons livres, $c_{\sigma \mathbf{k}}^{\dagger}$ ($c_{\sigma \mathbf{k}}$) descreve o operador de criação (aniquilação) de elétrons, σ é o spin e $\mathbf{k}$ é o número de onda.

$\mathcal{H}_{imp}$ descreve a impureza do sistema e pode ser escrita como

$$\mathcal{H}_{imp} = \sum_{\sigma} \epsilon_{d\sigma} d_{\sigma}^{\dagger} d_{\sigma}. \quad (2.34)$$

O primeiro termo representa a impureza de um único sítio; $\epsilon_{d\sigma}$ é a energia desses elétrons; $d_{\sigma}^{\dagger}$ (d_{σ}) representa o operador de criação (destruição) de elétrons no nível energético da impureza, o segundo termo descreve a repulsão de Coulomb para estados spins opostos. Os termos $n_{d\uparrow}$ e $n_{d\downarrow}$ são os operadores número $d_{\sigma}^{\dagger}d_{\sigma}$, o terceiro termo descreve a hibridização entre a impureza e o hospedeiro metálico e pode ser escrita como

$$\mathcal{H}_{hib} = \sum_{\sigma \mathbf{k}} \left(V_{\sigma \mathbf{k}} c_{\sigma \mathbf{k}}^{\dagger} d_{\sigma} + V_{\sigma \mathbf{k}}^{*} d_{\sigma}^{\dagger} c_{\sigma \mathbf{k}} \right), \quad (2.35)$$

em que $V_{\sigma \mathbf{k}}$, representa a intensidade de troca de elétrons dos estados da impureza com o hospedeiro.

2.4 Funções de Green

As funções de Green recebem esse nome em homenagem a George Green (1793-1841), seu criador. Seu formalismo é bastante utilizado para resolução de problemas que envolvem o estudo de equações diferenciais parciais e ordinárias, presentes em vários campos da física.

No desenvolvimento deste trabalho foi utilizada a função de Green retardada que pode ser escrita da seguinte forma

$$\mathcal{G}_{\sigma}^R(\mathbf{r}, t; \mathbf{r}', t') = -\frac{i}{\hbar} \theta(t - t') Z^{-1} \sum_n e^{-\beta E_n} \left\langle n \left| [\Psi_{\sigma}(\mathbf{r}, t), \Psi_{\sigma}^{\dagger}(\mathbf{r}', t')]_{+} \right| n \right\rangle, \quad (2.36)$$

onde $\theta(t - t')$ é a função degrau; Z é a função de partição do sistema; $[\dots, \dots]_{+}$ representa a operação de anticomutação. Os operadores $\Psi_{\sigma}^{\dagger}(\mathbf{r}', t')$ e $\Psi_{\sigma}(\mathbf{r}, t)$ descrevem a criação de uma partícula com spin σ na posição $\mathbf{r}'$ no instante t' e sua destruição na posição $\mathbf{r}$ e instante t , respectivamente. E, por fim, a média térmica $\langle \dots \rangle$ aplicada no anticomutador.

Até agora, foram apresentadas as funções de Green que encontram-se no domínio do tempo (t e t'). Porém, o objeto de estudo deste trabalho é a densidade de estados (DOS - densidades de estados), que é obtida através da parte imaginária da função de Green no domínio da energia,

$$\rho_{DOS}(\omega) = -\frac{1}{\pi} \text{Im} [\mathcal{G}_{\sigma}^R(\omega)], \quad (2.37)$$

sendo assim, a transformada de Fourier faz-se necessária. Com a utilização dessa ferramenta

matemática é possível mudar o domínio do tempo para o domínio da energia.

Assim como também é possível extrair algumas informações quando observa-se os polos encontrado para as funções, em que é possível determinar a energia da quasipartícula estudada. O que levaria a "localização" dessa quasipartícula, quando feito um paralelo com a física experimental e com as energias que são propriedades fundamentais da matéria.

Para resolução, a técnica normalmente utilizada é a equação de movimento (EOM - Equation of motion), que será melhor discutida na seção seguinte.

2.5 Equação de movimento

A equação de movimento (EOM) é uma técnica aplicada às funções de Green para determinar como se dá a evolução temporal dos operadores do sistema [41].

Abaixo está a função de Green retardada, os operadores estão em tempos distintos, t e 0 .

$$\mathcal{G}_{\Psi_i \Psi_j}^R(t, 0) = -\frac{i}{\hbar} \theta(t - 0) Z_e^{-1} \sum_n e^{-\beta E_n} \left\langle n \left| \left[\Psi_i(t), \Psi_j^\dagger(0) \right]_+ \right| n \right\rangle. \quad (2.38)$$

Agora é preciso fazer uma derivada temporal da função $\mathcal{G}^R$ para que se possa desenvolver o método da EOM.

$$\begin{aligned} \frac{\partial}{\partial t} \mathcal{G}_{\Psi_i \Psi_j}^R(t, 0) &= -\frac{i}{\hbar} \left(\frac{\partial}{\partial t} \theta(t - 0) \right) Z_e^{-1} \sum_n e^{-\beta E_n} \left\langle n \left| \left[\Psi_i(t), \Psi_j^\dagger(0) \right]_+ \right| n \right\rangle \\ &\quad - \frac{i}{\hbar} \theta(t - 0) Z_e^{-1} \sum_n e^{-\beta E_n} \left\langle n \left| \left[\left(\frac{\partial}{\partial t} \Psi_i(t) \right), \Psi_j^\dagger(0) \right]_+ \right| n \right\rangle, \end{aligned} \quad (2.39)$$

onde a derivada da função degrau corresponde a uma função delta de Dirac, $\frac{\partial}{\partial t} \theta(t - 0) = \delta(t - 0)$. Aplicando a equação de Heisenberg para resolver $\frac{\partial}{\partial t} \Psi_i(t)$, temos

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} \Psi_i(t) &= [\Psi_i, \mathcal{H}] \\ \frac{\partial}{\partial t} \Psi_i(t) &= -\frac{i}{\hbar} [\Psi_i, \mathcal{H}]. \end{aligned} \quad (2.40)$$

Resolvendo por meio da comutação do operador de aniquilação $\Psi_i(t)$ com o Hamiltoniano $\mathcal{H}$

total do sistema,

$$\begin{aligned}
\frac{\partial}{\partial t} \mathcal{G}_{\Psi_i \Psi_j}^R(t, 0) &= -\frac{i}{\hbar} \delta(t-0) Z_e^{-1} \sum_n e^{-\beta E_n} \left\langle n \left| \left[\Psi_i(t), \Psi_j^\dagger(0) \right]_+ \right| n \right\rangle \\
&\quad - \frac{i}{\hbar} \theta(t-0) Z_e^{-1} \sum_n e^{-\beta E_n} \left\langle n \left| \left[-\frac{i}{\hbar} [\Psi_i, \mathcal{H}], \Psi_j^\dagger(0) \right]_+ \right| n \right\rangle \\
&= -\frac{i}{\hbar} \delta(t-0) Z_e^{-1} \sum_n e^{-\beta E_n} \left\langle n \left| \left[\Psi_i(t), \Psi_j^\dagger(0) \right]_+ \right| n \right\rangle \\
&\quad - \left(-\frac{i}{\hbar} \right) \frac{i}{\hbar} \theta(t-0) Z_e^{-1} \sum_n e^{-\beta E_n} \left\langle n \left| \left[[\Psi_i, \mathcal{H}], \Psi_j^\dagger(0) \right]_+ \right| n \right\rangle. \quad (2.41)
\end{aligned}$$

O último termo assemelha-se a Eq. (2.38), então podemos reescrever a equação acima como

$$\begin{aligned}
\frac{\partial}{\partial t} \mathcal{G}_{\Psi_i \Psi_j}^R(t, 0) &= -\frac{i}{\hbar} \delta(t-0) Z_e^{-1} \sum_n e^{-\beta E_n} \left\langle n \left| \left[\Psi_i(t), \Psi_j^\dagger(0) \right]_+ \right| n \right\rangle \\
&\quad - \frac{i}{\hbar} \mathcal{G}_{[\Psi_i, \mathcal{H}] \Psi_j}^R(t, 0). \quad (2.42)
\end{aligned}$$

Aplicando agora, a transformada de Fourier para que se obtenha a função de Green no domínio da energia. A transformada de Fourier para a função de Green retardada é dada por

$$\tilde{\mathcal{G}}_{\Psi_i \Psi_j}^R(\omega^+) = \int_{-\infty}^{+\infty} dt \mathcal{G}_{\Psi_i \Psi_j}^R(t, 0) e^{\frac{i}{\hbar} \omega^+ t}, \quad (2.43)$$

em que, $\omega^+ = \omega + i\eta^+$ é a frequência espectral e $\eta^+ \rightarrow 0^+$.

Aplicando a propriedade de integração por partes na Eq. (2.43), obtêm-se

$$-\frac{i}{\hbar} \omega^+ \tilde{\mathcal{G}}_{\Psi_i \Psi_j}^R(\omega^+) = \int_{-\infty}^{+\infty} dt \frac{\partial}{\partial t} \mathcal{G}_{\Psi_i \Psi_j}^R(t, 0) e^{\frac{i}{\hbar} \omega^+ t}. \quad (2.44)$$

Substituindo a Eq. (2.42) na Eq. (2.44),

$$\begin{aligned}
-\frac{i}{\hbar} \omega^+ \tilde{\mathcal{G}}_{\Psi_i \Psi_j}^R(\omega^+) &= \int_{-\infty}^{+\infty} dt \left[-\frac{i}{\hbar} \delta(t-0) Z_e^{-1} \sum_n e^{-\beta E_n} \left\langle n \left| \left[\Psi_i(t), \Psi_j^\dagger(0) \right]_+ \right| n \right\rangle \right. \\
&\quad \left. - \frac{i}{\hbar} \mathcal{G}_{[\Psi_i, \mathcal{H}] \Psi_j}^R(t, 0) \right] e^{\frac{i}{\hbar} \omega^+ t} \\
&= -\frac{i}{\hbar} Z_e^{-1} \sum_n e^{-\beta E_n} \int_{-\infty}^{+\infty} dt \delta(t-0) \left\langle n \left| \left[\Psi_i(t), \Psi_j^\dagger(0) \right]_+ \right| n \right\rangle e^{\frac{i}{\hbar} \omega^+ t} \\
&\quad - \frac{i}{\hbar} \int_{-\infty}^{+\infty} dt \mathcal{G}_{[\Psi_i, \mathcal{H}] \Psi_j}^R(t, 0) e^{\frac{i}{\hbar} \omega^+ t}. \quad (2.45)
\end{aligned}$$

Substituindo $Z = \text{Tr} \{ e^{-\beta \mathcal{H}} \} = \sum_n e^{-\beta E_n}$ e $\int_{-\infty}^{+\infty} \delta(t - t_0) f(t) dt = f(t_0)$ no primeiro termo e utilizando o resultado da Eq. (2.44), a equação fica

$$\begin{aligned}
-\frac{i}{\hbar} \omega^+ \tilde{\mathcal{G}}_{\Psi_i \Psi_j}^R(\omega^+) &= -\frac{i}{\hbar} \left(\frac{1}{\sum_n e^{-\beta E_n}} \right) \sum_n e^{-\beta E_n} \left\langle n \left| \left[\Psi_i(0), \Psi_j^\dagger(0) \right]_+ \right| n \right\rangle e^{\frac{i}{\hbar} \omega^+ 0} \\
&\quad - \frac{i}{\hbar} \tilde{\mathcal{G}}_{[\Psi_i, \mathcal{H}] \Psi_j}^R(\omega^+) \\
-\frac{i}{\hbar} \omega^+ \tilde{\mathcal{G}}_{\Psi_i \Psi_j}^R(\omega^+) &= -\frac{i}{\hbar} \langle [\Psi_i(0), \Psi_j^\dagger(0)]_+ \rangle \langle n|1|n \rangle - \frac{i}{\hbar} \tilde{\mathcal{G}}_{[\Psi_i, \mathcal{H}] \Psi_j}^R(\omega^+),
\end{aligned} \tag{2.46}$$

este último termo é uma nova função de Green.

Sendo $\omega^+ = (\omega + i\eta)$ e $\langle n|n \rangle = 1$, a função de Green resulta em

$$(\omega + i\eta) \tilde{\mathcal{G}}_{\Psi_i \Psi_j}^R(\omega) = \langle [\Psi_i(0), \Psi_j^\dagger(0)]_+ \rangle + \tilde{\mathcal{G}}_{[\Psi_i, \mathcal{H}] \Psi_j}^R(\omega). \tag{2.47}$$

Quando calculamos funções de Green há sempre o surgimento de novas funções de Green como resultado e, assim, a realização de novos cálculos tornam-se necessários. Em alguns casos, não é possível chegar a um resultado fechado. Para esses casos, faz-se o uso de aproximações apropriadas para o sistema, a fim de evitar ao máximo a perda de informações do sistema físico e obter uma solução.

Uma outra abordagem para os cálculos das funções de Green pode ser utilizada. Essa seria a notação de Zubarev. Por ser mais objetiva, a notação de Zubarev foi utilizada [42].

$$\omega^+ \langle \langle \Psi_i; \Psi_j^\dagger \rangle \rangle = \langle [\Psi_i, \Psi_j^\dagger]_+ \rangle + \langle \langle [\Psi_i, \mathcal{H}]; \Psi_j^\dagger \rangle \rangle, \tag{2.48}$$

no qual $\langle \langle \Psi_i; \Psi_j^\dagger \rangle \rangle = \tilde{\mathcal{G}}_{\Psi_i \Psi_j}^R(\omega)$.

Capítulo 3

Modelo teórico

O modelo proposto é composto por uma impureza quântica (QI - quantum impurity) que acopla-se tanto a uma ponta spin polarizada com spin inteiro S quanto a um fio supercondutor topológico (TSC - topological super conductor). Estão localizados nas bordas do fio TSC os modos zero de Majorana (MZMs - Majorana-zero-modes) γ_1 e γ_2 , em que ε_M representa a superposição entre os estados de MZMs e $\lambda_{1(2)}$ o termo de hopping QI-TSC. Os MZMs, apesar de estarem espacialmente separados, comportam-se como um férmion não-local, representado pelo sítio fermiônico delocalizado f , que, por sua vez, possui um termo de acoplamento t com a QI e emparelhamento Δ do par de Cooper do tipo "p".

Com esta proposta é esperado mostrar uma excitação de quasipartícula do tipo Majorana-Ising (MIQ - Majorana-Ising quasiparticle) γ_{MIQ} localizada no sítio da QI. É possível observar um pico de condutância em zero $\mathcal{G}_{\text{MIQ}}(0) = \frac{e^2}{4h}$ para o γ_{MIQ} , quando satisfeitas algumas condições, mas a condutância total ainda é $\mathcal{G}_{\text{Total}}(0) = \frac{e^2}{2h}$. Isso ocorre quando um processo genuíno de tunelamento eletrônico está presente e há uma completa ausência de reflexão de Andreev local.

3.1 Hamiltoniano do sistema

O Hamiltoniano do sistema pode ser escrito como

$$\mathcal{H} = \sum_{k\alpha\sigma} \varepsilon_{k\alpha} c_{k\alpha\sigma}^\dagger c_{k\alpha\sigma} + \sum_{\sigma} \varepsilon_{\sigma} d_{\sigma}^\dagger d_{\sigma} + \sum_{k\alpha\sigma} (V c_{k\alpha\sigma}^\dagger d_{\sigma} + H.c.) + J s^z S^z + \mathcal{H}_{\text{MZM}}. \quad (3.1)$$

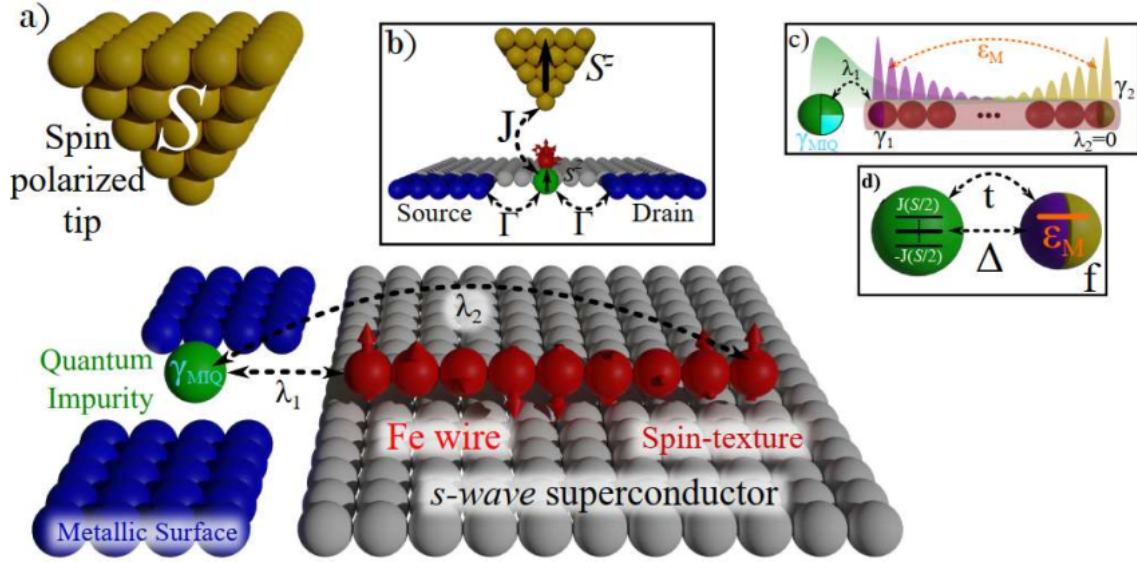


Figura 3.1: (a) Proposta de aparato experimental para a aparição da excitação MIQ. Composto por: uma ponta de spin polarizada (esferas amarelas) com spin interagente inteiro S , acoplada a uma QI de um único nível (esfera verde) com uma interação de troca do tipo Ising J , esta QI está flanqueada por dois terminais metálicos (source e drain - esferas azuis) e possuem um acoplamento terminal-QI, Γ ; a QI está acoplada a uma cadeia magnética helicoidal (esferas vermelhas) por um fator $\lambda_{1(2)}$ e depositada sobre uma superfície supercondutora do tipo "s" (esferas cinzas) que induz na cadeia helicoidal a supercondutividade do tipo "p". (b) Visão lateral do sistema. (c) Representação esquemática do sistema, que simula a fracionalização do férmion de Majorana γ_{MIQ} , ϵ_M representa o acoplamento entre os MZMs γ_1 e γ_2 (para esse caso, $\lambda_2 = 0$) que se encontram nas bordas do fio e as respectivas representações de suas funções de onda ao longo do fio. (d) Representação esquemática do férmion não-local f formado interagindo com a QI, com acoplamento t e emparelhamento do par de Cooper Δ . Adaptado de: Sanches, *et al.*, PRB 107,155144 (2023).

O primeiro termo descreve os terminais metálicos, $c_{k\alpha\sigma}^\dagger (c_{k\alpha\sigma})$ é o operador de criação (destruição), também conhecido como operador número e possui momento k , spin σ , energia $\varepsilon_{k\alpha}$ e α está associado aos terminais da direita e esquerda. O segundo termo está associado ao discreto de energia, que possui uma energia ε_σ . O terceiro termo descreve a hibridização entre o terminal metálico e a QI, sendo V a amplitude de acoplamento. O quarto termo descreve a interação dos spins, onde J é o termo de troca. O último termo está associado ao acoplamento da QI aos férmions de Majorana, que pode ser escrito como

$$\mathcal{H}_{MZM} = i\varepsilon_M \gamma_1 \gamma_2 + \lambda_1 (d_\uparrow - d_\uparrow^\dagger) \gamma_1 + \lambda_2 (d_\uparrow + d_\uparrow^\dagger) \gamma_2. \quad (3.2)$$

O primeiro termo da Eq. (3.2), descreve a interação entre os férmions de Majoranas e ε_M representa a amplitude desse acoplamento. Enquanto λ_1 e λ_2 são os parâmetros de acoplamento entre a QI e os férmions de Majoranas γ_1 e γ_2 , respectivamente.

Cada férmions de Majoranas pode ser escrito na forma de operadores fermiônicos. Então

$$\gamma_1 = \frac{1}{\sqrt{2}} (f^\dagger + f), \quad (3.3)$$

$$\gamma_2 = \frac{i}{\sqrt{2}} (f^\dagger - f). \quad (3.4)$$

Também podemos escrever λ_1 e λ_2 como

$$\lambda_1 = \frac{t + \Delta}{\sqrt{2}}, \quad (3.5)$$

$$\lambda_2 = i \left(\frac{\Delta - t}{\sqrt{2}} \right). \quad (3.6)$$

Quando λ_1 e λ_2 são escritos dessa forma, ganhamos um modelo mínimo de Kitaev. E, no caso dos férmions de Majoranas, sua partícula é igual a sua antipartícula, então $\gamma_1 = \gamma_1^\dagger$ e $\gamma_2 = \gamma_2^\dagger$. E por eles apresentarem a característica de um férmion não local, podemos escrevê-lo agora na base fermiônica $f = \frac{1}{\sqrt{2}} (\gamma_1 + i\gamma_2)$ e $f^\dagger = \frac{1}{\sqrt{2}} (\gamma_1 - i\gamma_2)$.

Reescrevendo o primeiro termo da Eq. (3.2) já na base fermiônica, temos

$$\begin{aligned}
i\varepsilon_M \gamma_1 \gamma_2 &= i\varepsilon_M \left[\frac{1}{\sqrt{2}}(f^\dagger + f) \frac{i}{\sqrt{2}}(f^\dagger - f) \right] \\
&= \frac{i^2 \varepsilon_M}{2} (f^\dagger + f)(f^\dagger - f) \\
&= -\frac{\varepsilon_M}{2} (f^\dagger + f)(f^\dagger - f) \\
&= -\frac{\varepsilon_M}{2} [f^\dagger(f^\dagger + f) + f(f^\dagger - f)] \\
&= -\frac{\varepsilon_M}{2} [f^\dagger f^\dagger - f^\dagger f + f f^\dagger - f f] \\
&= -\frac{\varepsilon_M}{2} (-f^\dagger f + f f^\dagger) \\
i\varepsilon_M \gamma_1 \gamma_2 &= -\frac{\varepsilon_M}{2} (-f^\dagger f + f f^\dagger). \tag{3.7}
\end{aligned}$$

O operador de anticomutação nos diz que

$$\begin{aligned}
[a_i, a_j^\dagger]_+ &= a_i a_j^\dagger + a_j^\dagger a_i \\
[a_i, a_j^\dagger]_+ &= \delta_{ij}. \tag{3.8}
\end{aligned}$$

Agora, aplicando a anticomutação em $[f, f^\dagger]_+$.

$$\begin{aligned}
[f, f^\dagger]_+ &= f f^\dagger + f^\dagger f = 1 \\
f f^\dagger &= 1 - f^\dagger f. \tag{3.9}
\end{aligned}$$

Substituindo a Eq. (3.9) na Eq. (3.7), temos

$$\begin{aligned}
i\varepsilon_M \gamma_1 \gamma_2 &= -\frac{\varepsilon_M}{2} (-f^\dagger f + f f^\dagger) \\
&= -\frac{\varepsilon_M}{2} (-f^\dagger f + 1 - f^\dagger f) \\
&= -\frac{\varepsilon_M}{2} (-2f^\dagger f + 1) \\
i\varepsilon_M \gamma_1 \gamma_2 &= \varepsilon_M \left(f^\dagger f - \frac{1}{2} \right). \tag{3.10}
\end{aligned}$$

A Eq. (3.10) nos diz que, agora, podemos escrever os férmions de Majoranas γ_1 e γ_2 como um férmion regular, apesar de estarem espacialmente separados.

Reescrevendo o segundo termo da Eq. (3.2) também na base fermiônica,

$$\begin{aligned}
\lambda_1 (d_\uparrow - d_\uparrow^\dagger) \gamma_1 &= \frac{\lambda_1}{\sqrt{2}} \left[d_\uparrow (f^\dagger + f) - d_\uparrow^\dagger (f^\dagger + f) \right] \\
&= \frac{\lambda_1}{\sqrt{2}} \left(d_\uparrow f^\dagger + d_\uparrow f - d_\uparrow^\dagger f^\dagger - d_\uparrow^\dagger f \right) \\
\lambda_1 (d_\uparrow - d_\uparrow^\dagger) \gamma_1 &= \frac{\lambda_1}{\sqrt{2}} \left(d_\uparrow f^\dagger + d_\uparrow f - d_\uparrow^\dagger f^\dagger - d_\uparrow^\dagger f \right). \tag{3.11}
\end{aligned}$$

Substituindo o valor de λ_1

$$\begin{aligned}
\lambda_1 (d_\uparrow - d_\uparrow^\dagger) \gamma_1 &= \frac{(t + \Delta)}{\sqrt{2}} \frac{1}{\sqrt{2}} \left(d_\uparrow f^\dagger + d_\uparrow f - d_\uparrow^\dagger f^\dagger - d_\uparrow^\dagger f \right) \\
&= \frac{1}{2} \left((t + \Delta) d_\uparrow f^\dagger + (t + \Delta) d_\uparrow f - (t + \Delta) d_\uparrow^\dagger f^\dagger - (t + \Delta) d_\uparrow^\dagger f \right) \\
\lambda_1 (d_\uparrow - d_\uparrow^\dagger) \gamma_1 &= \frac{1}{2} \left(t d_\uparrow f^\dagger + \Delta d_\uparrow f^\dagger + t d_\uparrow f + \Delta d_\uparrow f \right) \\
&\quad + \frac{1}{2} \left(-t d_\uparrow^\dagger f^\dagger - \Delta d_\uparrow^\dagger f^\dagger - t d_\uparrow^\dagger f - \Delta d_\uparrow^\dagger f \right). \tag{3.12}
\end{aligned}$$

Reescrevendo o terceiro termo da Eq. (3.2), temos

$$\begin{aligned}
\lambda_2 (d_\uparrow + d_\uparrow^\dagger) \gamma_2 &= \frac{i\lambda_2}{\sqrt{2}} \left(d_\uparrow (f^\dagger - f) + d_\uparrow^\dagger (f^\dagger - f) \right) \\
&= \frac{i\lambda_2}{\sqrt{2}} \left(d_\uparrow f^\dagger - d_\uparrow f + d_\uparrow^\dagger f^\dagger - d_\uparrow^\dagger f \right) \\
&= \frac{i\lambda_2}{\sqrt{2}} \left(d_\uparrow f^\dagger - d_\uparrow f + d_\uparrow^\dagger f^\dagger - d_\uparrow^\dagger f \right). \tag{3.13}
\end{aligned}$$

Substituindo agora o valor de λ_2 ,

$$\begin{aligned}
\lambda_2 (d_\uparrow + d_\uparrow^\dagger) \gamma_2 &= -\frac{1}{2} \left((\Delta - t) d_\uparrow f^\dagger - (\Delta - t) d_\uparrow f + (\Delta - t) d_\uparrow^\dagger f^\dagger - (\Delta - t) d_\uparrow^\dagger f \right) \\
\lambda_2 (d_\uparrow + d_\uparrow^\dagger) \gamma_2 &= -\frac{1}{2} \left(\Delta d_\uparrow f^\dagger - t d_\uparrow f^\dagger - \Delta d_\uparrow f + t d_\uparrow f \right) \\
&\quad - \frac{1}{2} \left(\Delta d_\uparrow^\dagger f^\dagger - t d_\uparrow^\dagger f^\dagger - \Delta d_\uparrow^\dagger f + t d_\uparrow^\dagger f \right). \tag{3.14}
\end{aligned}$$

Somando a Eq. (3.11) e Eq. (3.14), temos

$$\begin{aligned}
\lambda_1 (d_\uparrow - d_\uparrow^\dagger) \gamma_1 + \lambda_2 (d_\uparrow + d_\uparrow^\dagger) \gamma_2 &= \frac{1}{2} (td_\uparrow f^\dagger + \Delta d_\uparrow f^\dagger + td_\uparrow f + \Delta d_\uparrow f) \\
&+ \frac{1}{2} (-td_\uparrow^\dagger f^\dagger - \Delta d_\uparrow^\dagger f^\dagger - td_\uparrow^\dagger f - \Delta d_\uparrow^\dagger f) \\
&+ \frac{1}{2} (-\Delta d_\uparrow f^\dagger + td_\uparrow f^\dagger + \Delta d_\uparrow f - td_\uparrow f) \\
&+ \frac{1}{2} (-\Delta d_\uparrow^\dagger f^\dagger + td_\uparrow^\dagger f^\dagger + \Delta d_\uparrow^\dagger f - td_\uparrow^\dagger f) \\
&= \frac{1}{2} (2td_\uparrow f^\dagger + 2\Delta d_\uparrow f - 2\Delta d_\uparrow^\dagger f^\dagger - 2td_\uparrow^\dagger f) \\
&= td_\uparrow f^\dagger + \Delta d_\uparrow f - \Delta d_\uparrow^\dagger f^\dagger - td_\uparrow^\dagger f \\
\lambda_1 (d_\uparrow - d_\uparrow^\dagger) \gamma_1 + \lambda_2 (d_\uparrow + d_\uparrow^\dagger) \gamma_2 &= td_\uparrow f^\dagger + \Delta f^\dagger d_\uparrow^\dagger + tf d_\uparrow^\dagger + \Delta d_\uparrow f. \tag{3.15}
\end{aligned}$$

Na Eq. (3.2), temos a contribuição dos férmions de Majoranas para o Hamiltoniano escrito na base fermiônica.

$$\mathcal{H}_{MZM} = \varepsilon_M \left(f^\dagger f - \frac{1}{2} \right) + td_\uparrow f^\dagger + \Delta f^\dagger d_\uparrow^\dagger + tf d_\uparrow^\dagger + \Delta d_\uparrow f. \tag{3.16}$$

Reescrevendo a Eq. (3.16), temos

$$\mathcal{H}_{MZM} = \varepsilon_M f^\dagger f + \left(td_\uparrow f^\dagger + \Delta f^\dagger d_\uparrow^\dagger + \text{H.c.} \right). \tag{3.17}$$

Na Eq. (3.17), ε_M representa a energia de interação entre os férmions de Majorana (férmion não local f), t representa o termo de hopping que conecta os dois sítios e Δ representa a energia de ligação dos pares de Cooper.

3.2 Desenvolvimento das funções de Green

A partir do Hamiltoniano do sistema, as funções de Green podem ser determinadas por meio da técnica da EOM.

Utilizando a função de Green é possível saber como o sistema se comporta. Considerando

que o operador de spin-z é dado por $s^z = \frac{1}{2} \left(d_{\uparrow}^{\dagger} d_{\uparrow} - d_{\downarrow}^{\dagger} d_{\downarrow} \right) = \frac{1}{2} (n_{\uparrow} - n_{\downarrow})$, obtemos

$$\begin{aligned} \mathcal{H} &= \sum_{k\alpha\sigma} \varepsilon_{k\alpha} c_{k\alpha\sigma}^{\dagger} c_{k\alpha\sigma} + \sum_{\sigma} \varepsilon_{\sigma} d_{\sigma}^{\dagger} d_{\sigma} + \sum_{k\alpha\sigma} \left(V_{k\alpha} c_{k\alpha\sigma}^{\dagger} d_{\sigma} + H.c. \right) \\ &+ \frac{J}{2} \sum_m m n_{\uparrow} Y^{mm} - \frac{J}{2} \sum_m m n_{\downarrow} Y^{mm} \\ &+ \varepsilon_M f^{\dagger} f + t d_{\uparrow} f^{\dagger} + \Delta f^{\dagger} d_{\uparrow}^{\dagger} + t f d_{\uparrow}^{\dagger} + \Delta d_{\uparrow} f - \frac{\varepsilon_M}{2}, \end{aligned} \quad (3.18)$$

onde $Y^{mm} = |m\rangle\langle m|$.

A função de Green, no domínio da energia, na notação de Zubarev é dada por $\omega^+ \langle\langle A; B \rangle\rangle = \langle\{A, B\}\rangle + \langle\langle [A, \mathcal{H}]; B \rangle\rangle$, onde o primeiro termo representa a média térmica e do segundo termo surge uma nova equação de Green. Calculando $\langle\langle d_{\sigma}; d_{\sigma}^{\dagger} \rangle\rangle$, temos

$$\omega^+ \langle\langle d_{\sigma} Y^{mm}; d_{\sigma}^{\dagger} \rangle\rangle = \left\langle [d_{\sigma} Y^{mm}, d_{\sigma}^{\dagger}]_+ \right\rangle + \langle\langle [d_{\sigma} Y^{mm}, \mathcal{H}]; d_{\sigma}^{\dagger} \rangle\rangle, \quad (3.19)$$

com

$$\begin{aligned} \left\langle [d_{\sigma} Y^{mm}, d_{\sigma}^{\dagger}]_+ \right\rangle &= \langle (d_{\sigma} Y^{mm} d_{\sigma}^{\dagger} + d_{\sigma}^{\dagger} d_{\sigma} Y^{mm}) \rangle \\ &= \langle Y^{mm} (d_{\sigma} d_{\sigma}^{\dagger} + d_{\sigma}^{\dagger} d_{\sigma}) \rangle \\ &= \langle Y^{mm} \delta_{\sigma\sigma} \rangle \\ \left\langle [d_{\sigma} Y^{mm}, d_{\sigma}^{\dagger}]_+ \right\rangle &= \langle Y^{mm} \rangle. \end{aligned} \quad (3.20)$$

Do comutador, temos

$$\begin{aligned} [d_{\sigma} Y^{mm}, \mathcal{H}] &= \left[d_{\sigma} Y^{mm}, \sum_{k\alpha\sigma'} \varepsilon_{k\alpha} c_{k\alpha\sigma'}^{\dagger} c_{k\alpha\sigma'} \right] + [d_{\sigma} Y^{mm}, \varepsilon_1 (n_{\uparrow} + n_{\downarrow})] \\ &+ \left[d_{\sigma} Y^{mm}, \sum_{k\alpha\sigma'} \left(V_{k\alpha} c_{k\alpha\sigma'}^{\dagger} d_{\sigma'} + V_{k\alpha}^* d_{\sigma'}^{\dagger} c_{k\alpha\sigma'} \right) \right] \\ &+ \left[d_{\sigma} Y^{mm}, \frac{J}{2} \sum_m m n_{\uparrow} Y^{mm} \right] + \left[d_{\sigma} Y^{mm}, \left(-\frac{J}{2} \sum_m m n_{\downarrow} Y^{mm} \right) \right] \\ &+ [d_{\sigma} Y^{mm}, \mathcal{H}_{MZM}]. \end{aligned} \quad (3.21)$$

Resolvendo termo a termo o comutador e substituindo os resultados encontrados na Eq.

(3.2), temos

$$\begin{aligned}
\omega^+ \langle \langle d_\sigma Y^{mm}; d_\sigma^\dagger \rangle \rangle &= \langle Y^{mm} \rangle + \langle \langle \sum_{k\alpha\sigma'} V_{k\alpha}^* c_{k\alpha\sigma'} Y^{mm}; d_\sigma^\dagger \rangle \rangle \\
&+ \langle \langle \varepsilon_1 \delta_{\sigma\uparrow} d_\uparrow Y^{mm}; d_\sigma^\dagger \rangle \rangle + \langle \langle \varepsilon_1 \delta_{\sigma\downarrow} d_\downarrow Y^{mm}; d_\sigma^\dagger \rangle \rangle \\
&+ \langle \langle \frac{J}{2} \delta_{\sigma\uparrow} d_\uparrow m Y^{mm}; d_\sigma^\dagger \rangle \rangle + \langle \langle -\frac{J}{2} \delta_{\sigma\downarrow} d_\downarrow m Y^{mm}; d_\sigma^\dagger \rangle \rangle \\
&+ \langle \langle -\Delta f^\dagger Y^{mm} \delta_{\sigma\uparrow}; d_\sigma^\dagger \rangle \rangle + \langle \langle -t f Y^{mm} \delta_{\sigma\uparrow}; d_\sigma^\dagger \rangle \rangle
\end{aligned} \tag{3.22}$$

$$\begin{aligned}
\omega^+ \langle \langle d_\sigma Y^{mm}; d_\sigma^\dagger \rangle \rangle &= \langle Y^{mm} \rangle + \sum_{k\alpha\sigma'} V_{k\alpha}^* \langle \langle c_{k\alpha\sigma'} Y^{mm}; d_\sigma^\dagger \rangle \rangle \\
&+ \varepsilon_1 \delta_{\sigma\uparrow} \langle \langle d_\uparrow Y^{mm}; d_\sigma^\dagger \rangle \rangle + \varepsilon_1 \delta_{\sigma\downarrow} \langle \langle d_\downarrow Y^{mm}; d_\sigma^\dagger \rangle \rangle \\
&+ \frac{J}{2} \delta_{\sigma\uparrow} \langle \langle d_\uparrow m Y^{mm}; d_\sigma^\dagger \rangle \rangle - \frac{J}{2} \delta_{\sigma\downarrow} \langle \langle d_\downarrow m Y^{mm}; d_\sigma^\dagger \rangle \rangle \\
&+ -\Delta \delta_{\sigma\uparrow} \langle \langle f^\dagger Y^{mm}; d_\sigma^\dagger \rangle \rangle - t \delta_{\sigma\uparrow} \langle \langle f Y^{mm}; d_\sigma^\dagger \rangle \rangle.
\end{aligned} \tag{3.23}$$

Quando analisamos a Eq. (3.23) para o spin-up ($\sigma = \uparrow$) a equação fica

$$\begin{aligned}
(\omega^+ - \varepsilon_1 - \frac{Jm}{2}) \langle \langle d_\uparrow Y^{mm}; d_\uparrow^\dagger \rangle \rangle &= \langle Y^{mm} \rangle + \sum_{k\alpha\uparrow} V_{k\alpha}^* \langle \langle c_{k\alpha\uparrow} Y^{mm}; d_\uparrow^\dagger \rangle \rangle \\
&- \Delta \langle \langle f^\dagger Y^{mm}; d_\uparrow^\dagger \rangle \rangle - t \langle \langle f Y^{mm}; d_\uparrow^\dagger \rangle \rangle.
\end{aligned} \tag{3.24}$$

Resolvendo as Funções de Green (a resolução detalhada pode ser encontrada no apêndice A.1 deste trabalho) para o sistema, foram encontradas as seguintes equações

$$\begin{aligned}
(\omega^+ + i\Gamma) \langle \langle d_\sigma Y^{mm}; d_\sigma^\dagger \rangle \rangle &= \frac{1}{(2S+1)} \\
&+ \varepsilon_1 \delta_{\sigma\uparrow} \langle \langle d_\uparrow Y^{mm}; d_\sigma^\dagger \rangle \rangle + \varepsilon_1 \delta_{\sigma\downarrow} \langle \langle d_\downarrow Y^{mm}; d_\sigma^\dagger \rangle \rangle \\
&+ \frac{Jm}{2} \delta_{\sigma\uparrow} \langle \langle d_\uparrow Y^{mm}; d_\sigma^\dagger \rangle \rangle - \frac{Jm}{2} \delta_{\sigma\downarrow} \langle \langle d_\downarrow Y^{mm}; d_\sigma^\dagger \rangle \rangle \\
&- \Delta \delta_{\sigma\uparrow} \langle \langle f^\dagger Y^{mm}; d_\sigma^\dagger \rangle \rangle - t \delta_{\sigma\uparrow} \langle \langle f Y^{mm}; d_\sigma^\dagger \rangle \rangle;
\end{aligned} \tag{3.25}$$

$$(\omega^+ + \varepsilon_M) \langle \langle f^\dagger Y^{mm}; d_\sigma^\dagger \rangle \rangle = t \langle \langle d_\uparrow Y^{mm}; d_\sigma^\dagger \rangle \rangle - \Delta \langle \langle d_\uparrow Y^{mm}; d_\sigma^\dagger \rangle \rangle; \tag{3.26}$$

$$(\omega^+ - \varepsilon_M) \langle \langle f Y^{mm}; d_\sigma^\dagger \rangle \rangle = -t \langle \langle d_\uparrow Y^{mm}; d_\sigma^\dagger \rangle \rangle + \Delta \langle \langle d_\uparrow Y^{mm}; d_\sigma^\dagger \rangle \rangle; \tag{3.27}$$

$$\begin{aligned} \left(\omega^+ + \varepsilon_1 + \frac{Jm}{2} \right) \langle \langle d_{\uparrow}^{\dagger} Y^{mm}; d_{\sigma}^{\dagger} \rangle \rangle &= -i\Gamma \langle \langle d_{\sigma}^{\dagger} Y^{mm}; d_{\sigma}^{\dagger} \rangle \rangle \\ &+ t \langle \langle f^{\dagger} Y^{mm}; d_{\sigma}^{\dagger} \rangle \rangle + \Delta \langle \langle f Y^{mm}; d_{\sigma}^{\dagger} \rangle \rangle. \end{aligned} \quad (3.28)$$

Resolvendo para o spin-up. Escrevendo $\omega^+ = \omega + i\eta$, a equação fica

$$\begin{aligned} \left(\omega^+ - \varepsilon_1 - \frac{Jm}{2} + i\Gamma \right) \langle \langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \rangle \rangle &= \frac{1}{(2S+1)} 2t\Delta \left[\frac{(\omega + i\eta^+)}{\omega^2 - \varepsilon_M^2 + 2i\omega\eta^+ - (\eta^+)^2} \right] \langle \langle d_{\uparrow}^{\dagger} Y^{mm}; d_{\uparrow}^{\dagger} \rangle \rangle \\ &+ \left[\frac{\omega^+ (\Delta^2 + t^2) + \varepsilon_M (t^2 - \Delta^2)}{\omega^2 - \varepsilon_M^2 + 2i\omega\eta^+ - (\eta^+)^2} \right] \langle \langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \rangle \rangle. \end{aligned} \quad (3.29)$$

Fazendo as seguintes considerações,

$$K_+ = \frac{(\omega + i\eta^+) (\Delta^2 + t^2) + \varepsilon_M (t^2 - \Delta^2)}{\omega^2 - \varepsilon_M^2 + 2i\omega\eta^+ - (\eta^+)^2}, \quad (3.30)$$

$$K_- = \frac{(\omega + i\eta^+) (t^2 + \Delta^2) - \varepsilon_M (t^2 - \Delta^2)}{\omega^2 - \varepsilon_M^2 + 2i\omega\eta^+ - (\eta^+)^2}, \quad (3.31)$$

$$K_{MFs} = \frac{(\omega + i\eta^+)}{\omega^2 - \varepsilon_M^2 + 2i\omega\eta^+ - (\eta^+)^2}, \quad (3.32)$$

$$\tilde{K}_m = \frac{K_{MFs}}{(\omega^+ + \varepsilon_1 + \frac{Jm}{2} + i\Gamma - K_-)}, \quad (3.33)$$

e

$$\mathcal{R}_{MFs}^m = K_+ + (2t\Delta)^2 K_{MFs} \tilde{K}_m. \quad (3.34)$$

E agora substituindo estes termos nas equações, por fim, podemos encontrar $\langle \langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \rangle \rangle$, que é dada por

$$\langle \langle d_{\uparrow}; d_{\uparrow}^{\dagger} \rangle \rangle = \frac{1}{(2S+1)} \sum_m \frac{1}{(\omega^+ - \varepsilon_1 - \frac{Jm}{2} + i\Gamma - \mathcal{R}_{MFs}^m)}. \quad (3.35)$$

Analogamente, seguindo o mesmo protocolo, foram obtidas as demais funções de Green do

sistema.

Sendo,

$$K_m = \frac{K_{MFs}}{(\omega^+ - \varepsilon_1 - \frac{Jm}{2} + i\Gamma - K_+)} \quad (3.36)$$

$$\Upsilon_{MFs}^{-m} = K_- + (2t\Delta)^2 K_{MFs} K_m \quad (3.37)$$

$$\langle\langle d_\uparrow^\dagger; d_\uparrow \rangle\rangle = \frac{1}{2S+1} \sum_m \frac{1}{(\omega^+ + \varepsilon_1 + \frac{Jm}{2} + i\Gamma - \Upsilon_{MFs}^{-m})}; \quad (3.38)$$

$$\langle\langle d_\uparrow^\dagger; d_\uparrow^\dagger \rangle\rangle = -\frac{1}{(2S+1)} 2t\Delta \sum_m \frac{K_m}{(\omega^+ + \varepsilon_1 + \frac{Jm}{2} + i\Gamma - \Upsilon_{MFs}^{-m})}; \quad (3.39)$$

$$\langle\langle d_\uparrow; d_\uparrow \rangle\rangle = -\frac{1}{(2S+1)} 2\Delta t \sum_m \frac{\tilde{K}_m}{(\omega^+ - \varepsilon_1 - \frac{Jm}{2} + i\Gamma - \Upsilon_{MFs}^{+m})}. \quad (3.40)$$

3.3 Impureza quântica escrita na base de férmions de Majorana

A Impureza quântica (QI - quantum impurity) pode ser interpretada como um átomo artificial de um único nível. Sendo assim, pode ser reescrita como a combinação de dois férmions de Majorana.

Precisamos agora reescrever a QI também na base de férmions Majorana, γ_A e γ_B . Para isso, é necessário que determinemos as funções de Green $\langle\langle d_\sigma; d_\sigma^\dagger \rangle\rangle$ em operadores fermiônicos, que obedecem a relação $d_\uparrow = \frac{1}{\sqrt{2}} (\gamma_A + i\gamma_B)$ e $d_\uparrow^\dagger = \frac{1}{\sqrt{2}} (\gamma_A - i\gamma_B)$.

Então

$$\begin{aligned}
[d; d_\sigma^\dagger]_+ &= \left[\left\{ \frac{1}{\sqrt{2}} (\gamma_A(t) + i\gamma_B(t)) \right\}, \left\{ \frac{1}{\sqrt{2}} (\gamma_A(0) - i\gamma_B(0)) \right\} \right]_+ \\
&= \frac{1}{\sqrt{2}} (\gamma_A(t) + i\gamma_B(t)) \frac{1}{\sqrt{2}} (\gamma_A(0) - i\gamma_B(0)) + \frac{1}{\sqrt{2}} (\gamma_A(0) - i\gamma_B(0)) \frac{1}{\sqrt{2}} (\gamma_A(t) + i\gamma_B(t)) \\
&= \frac{1}{2} (\gamma_A(t)\gamma_A(0) - i\gamma_A(t)\gamma_B(0) + i\gamma_B(t)\gamma_A(0) - i^2\gamma_B(t)\gamma_B(0)) \\
&\quad + \frac{1}{2} (\gamma_A(0)\gamma_A(t) - i\gamma_A(0)\gamma_B(t) + i\gamma_B(0)\gamma_A(t) - i^2\gamma_B(0)\gamma_B(t)) \\
&= \frac{1}{2} [(\gamma_A(t)\gamma_A(0) + \gamma_A(0)\gamma_A(t)) - i(\gamma_A(t)\gamma_B(0) + \gamma_A(0)\gamma_B(t)) \\
&\quad + i(\gamma_B(t)\gamma_A(0) + \gamma_B(0)\gamma_A(t)) + (\gamma_B(t)\gamma_B(0) + \gamma_B(0)\gamma_B(t))] \\
[d; d_\sigma^\dagger]_+ &= \frac{1}{2} ([\gamma_A(t), \gamma_A(0)]_+ - i[\gamma_A(t), \gamma_B(0)]_+ + i[\gamma_B(t), \gamma_A(0)]_+ + [\gamma_B(t), \gamma_B(0)]_+) . \quad (3.41)
\end{aligned}$$

Então, a partir deste resultado, temos que

$$\langle\langle d_\sigma; d_\sigma^\dagger \rangle\rangle = \frac{1}{2} [\langle\langle \gamma_A; \gamma_A \rangle\rangle - i\langle\langle \gamma_A; \gamma_B \rangle\rangle + i\langle\langle \gamma_B; \gamma_A \rangle\rangle + \langle\langle \gamma_B; \gamma_B \rangle\rangle] . \quad (3.42)$$

Agora, calculando o primeiro e o último termo e escrevendo-os na base fermiônica, temos

$$\begin{aligned}
[\gamma_A, \gamma_A]_+ &= \left[\frac{1}{\sqrt{2}} (d_\uparrow^\dagger + d_\uparrow), \frac{1}{\sqrt{2}} (d_\uparrow^{\dagger'} + d_\uparrow') \right]_+ \\
&= \frac{1}{\sqrt{2}} (d_\uparrow^\dagger + d_\uparrow) \frac{1}{\sqrt{2}} (d_\uparrow^{\dagger'} + d_\uparrow') + \frac{1}{\sqrt{2}} (d_\uparrow^{\dagger'} + d_\uparrow') \frac{1}{\sqrt{2}} (d_\uparrow^\dagger + d_\uparrow) \\
&= \frac{1}{2} [(d_\uparrow^\dagger + d_\uparrow) (d_\uparrow^{\dagger'} + d_\uparrow') + (d_\uparrow^{\dagger'} + d_\uparrow') (d_\uparrow^\dagger + d_\uparrow)] \\
&= \frac{1}{2} [d_\uparrow^\dagger d_\uparrow^{\dagger'} + d_\uparrow^\dagger d_\uparrow' + d_\uparrow d_\uparrow^{\dagger'} + d_\uparrow d_\uparrow' + d_\uparrow^{\dagger'} d_\uparrow^\dagger + d_\uparrow^{\dagger'} d_\uparrow + d_\uparrow' d_\uparrow^\dagger + d_\uparrow' d_\uparrow] \\
&= \frac{1}{2} [(d_\uparrow^\dagger d_\uparrow^{\dagger'} + d_\uparrow^{\dagger'} d_\uparrow^\dagger) + (d_\uparrow^\dagger d_\uparrow' + d_\uparrow' d_\uparrow^\dagger) + (d_\uparrow d_\uparrow^{\dagger'} + d_\uparrow^{\dagger'} d_\uparrow) + (d_\uparrow d_\uparrow' + d_\uparrow' d_\uparrow)] \\
&= \frac{1}{2} [\langle\langle [d_\uparrow^\dagger, d_\uparrow^{\dagger'}]_+ \rangle\rangle + \langle\langle [d_\uparrow^\dagger, d_\uparrow']_+ \rangle\rangle \\
&\quad + \langle\langle [d_\uparrow, d_\uparrow^{\dagger'}]_+ \rangle\rangle + \langle\langle [d_\uparrow, d_\uparrow']_+ \rangle\rangle] . \quad (3.43)
\end{aligned}$$

Sabendo que os novos anticomutadores dão “origem” a novas funções de Green, temos que

$$\langle\langle [\gamma_A; \gamma_A]_+ \rangle\rangle = \frac{1}{2} [\langle\langle d_\uparrow^\dagger; d_\uparrow^{\dagger'} \rangle\rangle + \langle\langle d_\uparrow^\dagger; d_\uparrow' \rangle\rangle + \langle\langle d_\uparrow; d_\uparrow^{\dagger'} \rangle\rangle + \langle\langle d_\uparrow; d_\uparrow' \rangle\rangle] \quad (3.44)$$

Então, analogamente

$$\langle\langle\gamma_B;\gamma_B\rangle\rangle = \frac{1}{2}\left(-\langle\langle d_{\uparrow}^{\dagger};d_{\uparrow}^{\dagger}\rangle\rangle+\langle\langle d_{\uparrow}^{\dagger};d_{\uparrow}\rangle\rangle+\langle\langle d_{\uparrow};d_{\uparrow}^{\dagger}\rangle\rangle-\langle\langle d_{\uparrow};d_{\uparrow}\rangle\rangle\right), \quad (3.45)$$

$$\langle\langle\gamma_A;\gamma_B\rangle\rangle = \frac{i}{2}\left(\langle\langle d_{\uparrow}^{\dagger};d_{\uparrow}^{\dagger}\rangle\rangle-\langle\langle d_{\uparrow}^{\dagger};d_{\uparrow}\rangle\rangle+\langle\langle d_{\uparrow};d_{\uparrow}^{\dagger}\rangle\rangle-\langle\langle d_{\uparrow};d_{\uparrow}\rangle\rangle\right), \quad (3.46)$$

$$\langle\langle\gamma_B;\gamma_A\rangle\rangle = \frac{i}{2}\left(\langle\langle d_{\uparrow}^{\dagger};d_{\uparrow}^{\dagger}\rangle\rangle+\langle\langle d_{\uparrow}^{\dagger};d_{\uparrow}\rangle\rangle-\langle\langle d_{\uparrow};d_{\uparrow}^{\dagger}\rangle\rangle-\langle\langle d_{\uparrow};d_{\uparrow}\rangle\rangle\right). \quad (3.47)$$

Capítulo 4

Resultados e Discussão

4.1 Quasipartícula do tipo Majorana-Ising

4.1.1 Condutância

Podemos observar na Fig. 4.1, a condutância total para a QI, dada por $\mathcal{G}_{\text{Total}} = \mathcal{G}_{\text{ET}} + \mathcal{G}_{\text{LAR}}$, $\mathcal{G}_{\text{ET}}$ representa a contribuição do transporte eletrônico (ET - electronic transport) e $\mathcal{G}_{\text{LAR}}$ a contribuição da reflexão local de Andreev (LAR - local Andreev reflection) em função da tensão eV/Γ . Na Fig. 4.1(a), consideramos o caso em que o fio TSC é infinito ($\varepsilon_M = 0$) e o spin está desligado ($S=0$).

Este caso apresenta um pico de voltagem em zero (zero bias-peak - ZBP) na condutância dado por $\mathcal{G}_{\text{Total}}(0) = \frac{e^2}{2h}$ [3,4], que representa o MZM isolado γ_1 . Esse MZM, que se encontrava na borda do fio TSC, vaza em direção ao sítio da QI, agora como MZM γ_A . Após esse vazamento, a densidade de estados da QI é caracterizada por $\text{DOS}(\uparrow)[\gamma_A](0) = 1$ e $\text{DOS}(\uparrow)[\gamma_B](0) = 0$. Porém, é possível perceber a aparição de picos satélites na Fig. 4.1(a) que são resultado da divisão decorrente da condição $i\sqrt{2}\lambda_1\gamma_B\gamma_1$ dada pela Eq. (3.17).

Nossa proposta é isolar uma quasipartícula no sítio da QI e ainda obter uma condutância total $\mathcal{G}_{\text{Total}}(0) = \frac{e^2}{2h}$ para um fio TSC finito. Nesta configuração, essa excitação surge, como uma interação do tipo Ising. Porém, para que isso aconteça, é necessário que um spin inteiro S seja acoplado a QI com um valor específico (sweet spot) para a interação de troca J . É interessante frisar que o valor de J é muito específico para cada valor de spin analisado, ou seja, para que a MIQ seja observada é necessário que a análise seja feita para o valor determinado de S e J respectivo, qualquer alteração no valor de spin levaria a um novo valor de J para que a MIQ

pudesse ser observada novamente.

Com essas condições satisfeitas, verificamos que essa configuração corresponde ao isolamento de um MZM distinto, γ_B , que apresenta um pico ressonante caracterizado pelo peso espectral $\text{DOS}(\uparrow)[\gamma_B](0) = 1/2$, enquanto para γ_A temos a mesma amplitude, ou seja, $\text{DOS}(\uparrow)[\gamma_A](0) = 1/2$, mas com um vale no lugar.

Agora, consideramos a presença de um spin inteiro S . Fig. 4.1(c) e (d) mostram a condutância total na presença de $S=3$ e $J_h = 1.335\Gamma$ [veja a inserção b)-I da Fig. 4.2] para um TSC finito com $\varepsilon_M = \Gamma$. A condutância ZBP na Fig. 4.1(c) é $\mathcal{G}_{\text{Total}}(0) = \frac{e^2}{2h}$ como esperado, mas a decomposição nos canais ET e LAR descrita na Fig. 4.1(d) revela um resultado surpreendente: somente o ET se manifesta, enquanto a LAR é completamente suprimida na voltagem zero. Abaixo, verificaremos que a supressão da LAR corresponde a uma localização de quasi-partícula na DOS para γ_B , o que leva a $\text{DOS}(\uparrow)[\gamma_B](0) = 1/2$. Sendo assim, essa DOS finita contribui para uma condutância $\mathcal{G}_{\gamma_B}(0) = \mathcal{G}_{\text{MIQ}}(0) = \frac{e^2}{4h}$, onde definimos o MIQ $\gamma_B \equiv \gamma_{\text{MIQ}}$.

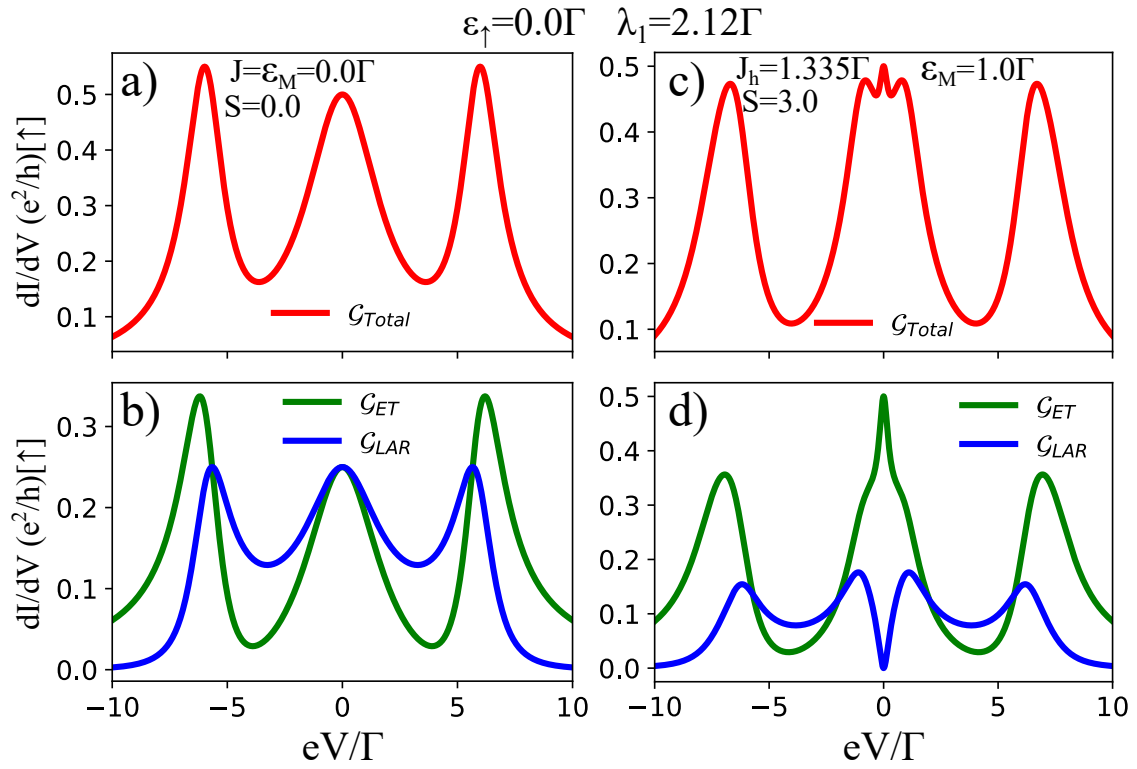


Figura 4.1: (a) Condutância total $\mathcal{G}_{\text{Total}}$ versus voltagem dos terminais do sistema eV em unidades do acoplamento Γ com MZMs isolados γ_1 e γ_2 ($\varepsilon_M = 0$) na ausência da ponta spin polarizada ($S=0$) e interação de troca J . (b) Contribuições das partes eletrônica e de Andreev local (iguais) para o ZBP. (c) Condutância total na QI para o sweet spot. Uma ponta spin polarizada é adicionada ao sistema com $S=3$ e interação de troca para o ponto especial (sweet spot) $J = J_h = 1.335\Gamma$ para um fio finito ($\varepsilon_M = 1\Gamma$), uma amplitude $\mathcal{G}_{\text{Total}}(0) = \frac{e^2}{2h}$ ainda é observada e aponta a existência da MIQ γ_{MIQ} no interior da QI. (d) No regime de (c), $\mathcal{G}_{\text{LAR}}(0)$ vai a zero e somente o termo $\mathcal{G}_{\text{ET}}(0)$ contribui para o ZBP. Retirado de: Sanches, *et al.*, PRB 107,155144 (2023).

4.1.2 Excitação de quasipartícula do tipo Majorana-Ising e seus perfis espectrais

Para entender o surgimento da MIQ, começamos com o caso trivial na Fig. 4.2(a): o painel central discrimina a DOS($\uparrow$) eletrônica nas respectivas DOSs para γ_A e γ_B , com $S=0$ e $\varepsilon_M = \Gamma$. Esse caso é considerado trivial, pois verificamos que em ambas as DOSs, γ_A e γ_B , estados ressonantes fixados em energia zero $\omega = 0$ estão presentes.

O estado fermiônico da QI pode ser ilustrado como uma esfera formada por dois MZMs representados por duas semi-esferas. Essa representação foi escolhida para ilustrar os dois estados ressonantes de energia zero (MZMs) nas DOSs γ_A e γ_B . Este esboço pode ser encontrado na inserção superior-direita da Fig. 4.2(a), onde cada calota ilustra o caráter “meio fermiônico” do

MZM, que corresponde a um MZM com $\text{DOS}(\uparrow)[\gamma_j](0) = 1$. A soma desses dois MZMs levam ao pico de condutância na energia zero $\mathcal{G}_{\text{Total}}(0) = \frac{e^2}{h}$. Os picos satélites na $\text{DOS}(\uparrow)[\gamma_B]$ ocorrem devido à superposição entre os MZMs γ_B e γ_1 .

Por outro lado, o painel de inserção a)-II da Fig. 4.2(a) mostra o canal de spin-down, que está desacoplado do TSC. Para analisá-lo sob a mesma perspectiva do canal de spin-up assumimos artificialmente $\varepsilon_{\downarrow} = 0$ e verificamos que ambos os MZMs, γ_C e γ_D , são identificados como estados ressonantes degenerados. A análise das DOSs para a componente de spin-down é semelhante à análise feita para as funções de Green da componente spin-up, porém ignorando os termos supercondutores. Como nenhum desses MZMs se superpõe ao fio, as assinaturas desses MZMs manifestam-se nos perfis das DOSs γ_C e γ_D . Devido a isso, picos satélites não emergem.

Já para o caso em que $\varepsilon_M = 0$, representado na inserção a)-I da Fig. 4.2(a), corresponde à situação não superposta entre γ_1 e γ_2 . Esse cenário é o ideal e contém os pilares para o comportamento da condutância da Fig. 4.1(a). É possível perceber que γ_B superpõe-se a γ_1 levando à picos satélites nas $\text{DOS}(\uparrow)[\gamma_B]$ e $\text{DOS}(\uparrow)[\gamma_B](0) = 0$, enquanto γ_A está isolado e localizado como um modo ressonante bem definido com peso espectral $\text{DOS}(\uparrow)[\gamma_A](0) = 1$. Portanto, $\mathcal{G}_{\text{Total}}(0) = \mathcal{G}_{\gamma_A}(0) = \frac{e^2}{2h}$. Esse caso é bem conhecido na literatura [3, 4] e aponta que o MZM γ_A contribui para a condutância como um estado ressonante, em contraste com γ_B , que mostra $\text{DOS}(\uparrow)[\gamma_B](0) = 0$. Isso impede uma condutância finita, ou seja, $\mathcal{G}_{\gamma_B}(0) = 0$.

Ao ligar o termo de troca J para um dado S , os perfis espectrais da $\text{DOS}(\uparrow)[\gamma_A]$ e $\text{DOS}(\uparrow)[\gamma_B]$ exibirão uma estrutura multi-nível. Além disso, essas densidades serão responsáveis, de acordo com a equação $\mathcal{G}_{\gamma_j}(\text{eV}) = \frac{e^2}{4h}[\text{DOS}(\uparrow)[\gamma_j](\text{eV}/2) + \text{DOS}(\uparrow)[\gamma_j](\text{-eV}/2)]$, por uma $\mathcal{G}_{\text{Total}}(0) \neq \frac{e^2}{h}$ não quantizada na equação $\mathcal{G}_{\text{Total}} = \mathcal{G}_{\gamma_A} + \mathcal{G}_{\gamma_B}$. Na situação de J arbitrário, as contribuições para $\mathcal{G}_{\text{Total}}(0) \neq 0$ não surgirão de estados ressonantes de modo zero bem definidos em $\text{DOS}(\uparrow)[\gamma_A]$ e $\text{DOS}(\uparrow)[\gamma_B]$. A localização do férmion de Majorana dentro do QI como um estado de modo zero ressonante ocorrerá apenas para o ponto específico $J = J_h$.

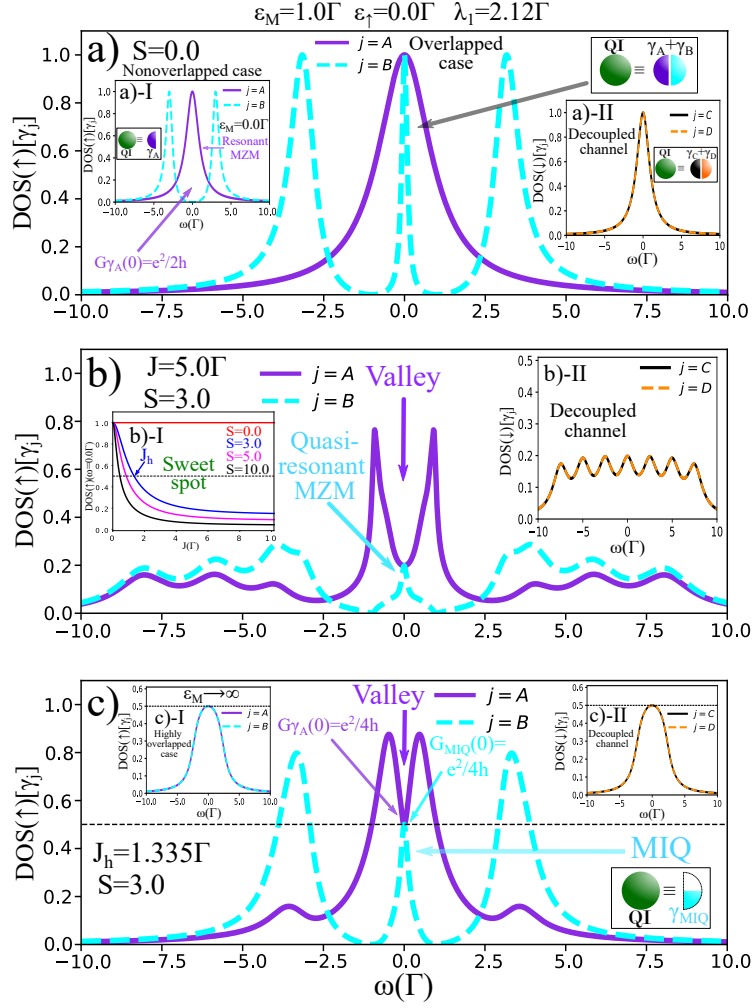


Figura 4.2: (a) O painel central mostra a dependência na frequência das DOSs normalizadas para os MZMs γ_A e γ_B para o canal do spin-up dentro da QI, assumindo que a ponta spin polarizada não está presente, assim como os MZMs γ_1 e γ_2 superpostos ($\varepsilon_M = 1\Gamma$) no TSC. Em cada DOS é possível encontrar um MZM ressonante, que corresponde a um meio férmion no sítio da QI representada como uma esfera verde na inserção, no canto superior direito. Esta esfera possui MZMs em seu interior representado pelas calotas para denotar a natureza de meio férmion do MZM. Na situação em que não há a superposição, apenas a calota γ_A permanece, [inserção a)-I]. O que leva a $\mathcal{G}_{\text{Total}}(0) = \mathcal{G}_{\gamma_A}(0) = \frac{e^2}{2h}$ na Fig. 4.1(a). Para o canal spin- down, que está desacoplado do TSC os MZMs γ_C e γ_D permanecem emparelhados dentro da QI [inset a)-II]. (b) Na presença de $S = 3$ e $J = 5\Gamma$ para $\varepsilon_M = 1\Gamma$ a DOS para γ_A muda drasticamente, exibindo um vale em $\omega = 0$ no lugar de um pico, enquanto para γ_B , o modo zero não é bem definido. Para restaurar o ZBP $\mathcal{G}_{\text{Total}}(0) = \frac{e^2}{2h}$ devemos escolher o valor correto de J para um dado S , i.e., o ponto especial $J = J_h$ [painel b)-I para a QI, a DOS da Eq. $\text{DOS}(\uparrow) = \frac{1}{2}(\text{DOS}(\uparrow)[\gamma_A] + \text{DOS}(\uparrow)[\gamma_B])$ impondo $\text{DOS}(\uparrow)(0) = 1/2$]. No canal de spin-down, as DOSs de γ_C e γ_D tornam-se degeneradas com uma estrutura com $2S + 1$ níveis, [painel b)-II]. (c) A escolha de $J = J_h = 1.335\Gamma$ de $S = 3$ define os vales e os picos para as DOSs γ_A e γ_B , respectivamente, onde introduzimos $\gamma_B \equiv \gamma_{\text{MIQ}}$ como sendo a quasipartícula do tipo Majorana-Ising, uma vez que, o pico representa um único MZM isolado no sistema. É caracterizado por um ZBP dado por $\mathcal{G}_{\text{MIQ}}(0) = \frac{e^2}{4h}$ ilustrado pela meia esfera na inserção, canto inferior direito, para a esfera verde representando o estado fermiônico da QI. Entretanto, $\mathcal{G}_{\text{Total}}(0) = \mathcal{G}_{\gamma_A}(0) + \mathcal{G}_{\text{MIQ}}(0) = \frac{e^2}{2h}$. Retirado de: Sanches, *et al.*, PRB 107,155144 (2023).

A Fig. 4.2(b) aborda a presença de um spin inteiro acoplado à QI para $\varepsilon_M = \Gamma$. Como podemos notar, a interação de Ising $J = 5\Gamma$ para $S = 3$ afeta claramente os perfis espectrais de $\text{DOS}(\uparrow)[\gamma_A]$ e $\text{DOS}(\uparrow)[\gamma_B]$. Basicamente, introduz uma estrutura multi-nível para os picos satélites e modifica drasticamente a localização do MZM em torno da voltagem zero. Surpreendentemente, a $\text{DOS}(\uparrow)[\gamma_A]$ apresenta um vale na energia zero e um MZM quasi-ressonante surge em $\text{DOS}(\uparrow)[\gamma_B]$. De fato, esta última não pode ser considerada um MZM ressonante bem definido: seu peso espectral não é exatamente um número inteiro ou semi-inteiro, e o alargamento da curva não segue a forma do tipo lorentziana. O tipo de curva dessas densidades espectrais são, então, distintas, mas contraintuitivamente, seus valores de voltagem em zero coincidem, ou seja, $\text{DOS}(\uparrow)[\gamma_A](0) = \text{DOS}(\uparrow)[\gamma_B](0)$.

Como o canal spin-up da QI é aquele acoplado ao TSC, os perfis espectrais na $\text{DOS}(\uparrow)[\gamma_A]$ e $\text{DOS}(\uparrow)[\gamma_B]$ não seguem estritamente a teoria do momento angular padrão para o desdobramento de Zeeman. Geralmente, essa teoria assegura que para um S inteiro, $2S$ níveis simetricamente deslocados em torno do correspondente em $\omega = \varepsilon_\uparrow = 0$ devem emergir. Aqui, de fato observamos um conjunto de simetria de espelho com S bandas de energia abaixo e acima do pico em zero, respectivamente, onde estruturas espectrais peculiares próximas surgem. Revelamos que os perfis diferem significativamente nessa faixa, como consequência da interação não trivial entre o TSC e o termo de troca Ising.

Na Fig. 4.3(d)-(f) podemos perceber que a manifestação desse efeito está dentro de uma região compreendida por paredes em formato de cone, abrangendo ω e ε_M nas DOSs do sistema. Dentro do cone, o efeito Zeeman torna-se incomum e o espaçamento de energia entre os níveis é simultaneamente governado por J e ε_M . Além disso, apenas o canal de spin-down mostra efeito Zeeman padrão, já que ele não interage com o TSC. Isso pode ser verificado no painel de inserção b)-II da Fig. 4.2(b), onde as DOSs para γ_C e γ_D , como esperado, apresentam a estrutura multi-nível $2S + 1$ ordinária garantida pela relação troca $J S^z S^z$ presente na Eq. (3.1).

Ressaltamos que ao diminuir o parâmetro de troca J , a restauração da condutância $\mathcal{G}_{\text{Total}}(0) = \frac{e^2}{2h}$ ainda pode ser permitida. Portanto, devemos lembrar que tal condutância surge do cumprimento da condição $\text{DOS}(\uparrow)(0) = 1/2$. Particularmente na inserção b)-I da Fig. 4.2(b), mostramos exatamente os pontos onde isso acontece considerando vários valores de S e $\varepsilon_M \neq 0$.

Particularmente, para $S = 3$, esse ponto especial, ocorre para $J = J_h = 1.335\Gamma$ e sua dependência em ε_M é revelada como muito fraca. Significa que $J = J_h = 1.335\Gamma$ ainda mantém o valor $\text{DOS}(\uparrow)(0) = 1/2$ enquanto ε_M não exceder muito Γ ($\varepsilon_M \gg \Gamma$). Falando experimental-

mente, J pode ser ajustado mudando a distância vertical entre a ponta e a QI. Assim, para $\varepsilon_M \neq 0$, $\mathcal{G}_{\text{Total}}(0)$ cai de $\frac{e^2}{h}$ para $\frac{e^2}{2h}$ quando $J = J_h$. Portanto, no ponto especial, se alguém souber previamente o spin S da ponta, J_h pode ser extraído da Fig. 4.2b)-I ou vice-versa.

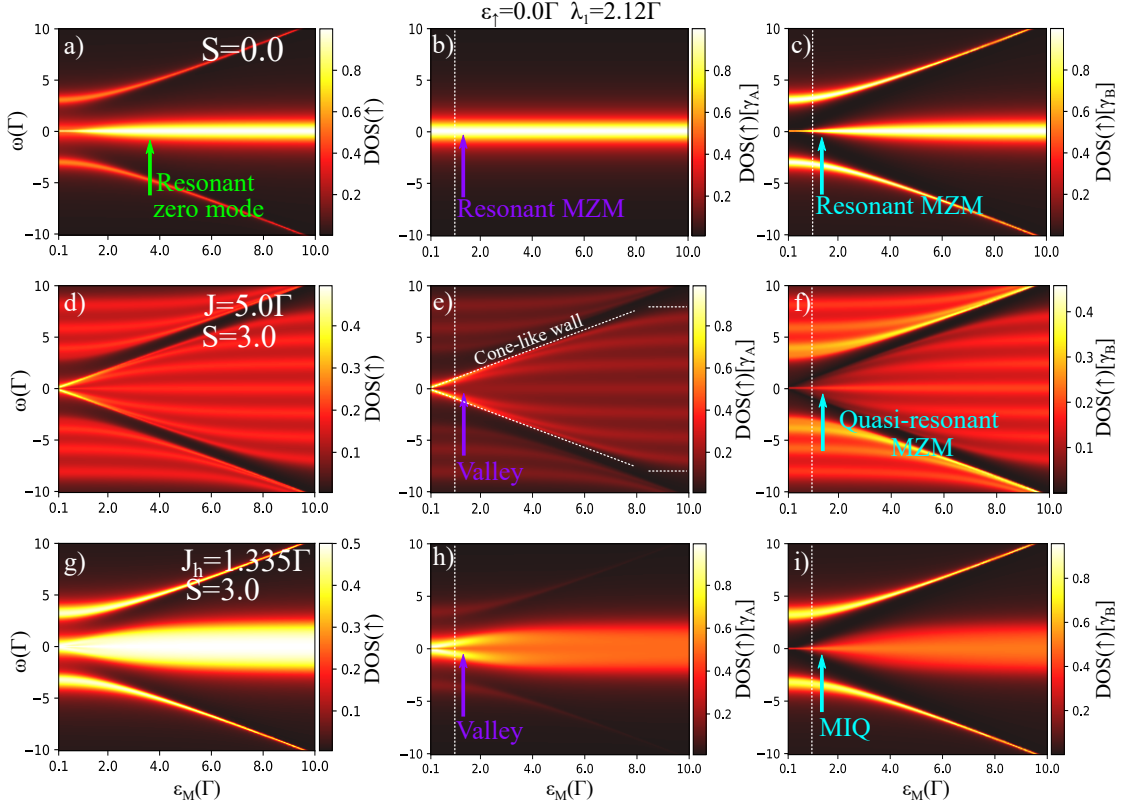


Figura 4.3: Mapa de cores das DOSs, eletrônica e de MZMs, para a QI, γ_A e γ_B , respectivamente: (a) Para o caso $S=0$, o ZBP na $DOS(\uparrow)$ emerge dos ZBPs individuais encontrados na $DOS(\uparrow)[\gamma_A]$ [painel(b)] e $DOS(\uparrow)[\gamma_B]$ [painel(c)], devido aos MZMs γ_A e γ_B que compõem a QI ($\varepsilon_\uparrow = 0$). Isso revela que o sistema não contém MZMs isolados e que o acoplamento entre γ_1 e γ_2 divide o modo de energia zero, levando ao aparecimento dos picos superiores e inferiores presentes nos painéis (a) e (c). Os painéis (d)-(f) expressam a influência de $S = 3$ e $J = 5\Gamma$ na QI, onde é possível perceber uma estrutura com $2S + 1$ níveis centrada em $\omega = 0$. Os picos superiores e inferiores mostram $2S$ níveis, cada. A região central de (e) possui uma estrutura do tipo vale em contraste à (f), que aponta um MZM quase ressonante. Nos dois casos, a estrutura com $2S + 1$ níveis é definida por paredes com formato de cone, até um limiar em ε_M . Neste caso, o TSC não atua e os MZMs γ_A e γ_B permanecem emparelhados (a)-(c). Os painéis (g)-(i) mostram os resultados para o ponto específico $J = J_h = 1.335\Gamma$, onde é possível perceber o pico e o vale na frequência zero muito bem resolvidos na $DOS(\uparrow)[\gamma_A]$ e $DOS(\uparrow)[\gamma_B]$, respectivamente. No painel (i) é possível perceber que o MIQ emerge da fusão das estruturas que constituem os $2S + 1$ níveis centrados em $\omega = 0$ ao diminuir o acoplamento J . Retirado de: Sanches, *et al.*, PRB 107,155144 (2023).

Na Fig. 4.2(c), apresentamos o caso $J = J_h = 1.335\Gamma$, que leva à nossa principal descoberta: a localização de um estado ressonante em energia zero na $DOS(\uparrow)[\gamma_B]$, com peso espectral $DOS(\uparrow)[\gamma_B](0) = \frac{1}{2}$. Essa amplitude indica que o MZM comum agora se encontra fra-

cionalizado e o valor da $\text{DOS}(\uparrow)[\gamma_B](0) = 1$ não está mais presente. Esse MZM fracionalizado, chamado de MIQ, leva a uma condutância $\mathcal{G}_{\gamma_B}(0) = \mathcal{G}_{\text{MIQ}}(0) = \frac{e^2}{4h}$, como garantido pela equação $\mathcal{G}_{\gamma_j}(\text{eV}) = \frac{e^2}{4h}[\text{DOS}(\uparrow)[\gamma_j](\text{eV}/2) + \text{DOS}(\uparrow)[\gamma_j](\text{eV}/2)]$. O valor $\text{DOS}(\uparrow)[\gamma_B](0) = 1/2$ pode ser visualizado de forma ilustrativa pela semi-esfera encontrada na inserção, no canto inferior direito da Fig. 4.2(c), que simboliza a fracionalização do MZM dentro do estado da QI. No entanto, para completar a condutância total $\mathcal{G}_{\text{Total}}(0) = \frac{e^2}{2h}$, o valor em energia zero da $\text{DOS}(\uparrow)[\gamma_A](0)$ deve coincidir, ou seja, $\text{DOS}(\uparrow)[\gamma_A](0) = 1/2$ e, como resultado, $\mathcal{G}_{\gamma_A}(0) = \frac{e^2}{4h}$ também. Aqui, enfatizamos que em $\text{DOS}(\uparrow)[\gamma_A](0)$ uma interferência quântica destrutiva manifesta-se e um estado ressonante não surge na energia zero.

Também, é importante esclarecer o mecanismo subjacente para produzir a MIQ, em que, a ideia chave é diminuir J , forçando assim a fusão das bandas laterais $2S$ (picos secundários) do sistema em direção à energia zero, onde um nível ressonante está fixado. Como resultado, essa soma de amplitudes para os picos secundários interfere construtivamente na energia zero, resultando em $\text{DOS}(\uparrow)(0) = 1/2$ para $J = J_h$. Além disso, nossas descobertas não dependem do sinal de J e, no caso de um spin semi-inteiro, a estrutura de múltiplos níveis é par e uma energia zero está ausente no espectro. Dessa forma, a MIQ não pode ser excitada.

Em relação às inserções c)-I e c)-II da Fig. 4.2, verificamos que, para $\varepsilon_M \gg \Gamma$ (ou $\varepsilon_M \rightarrow \infty$), as DOSs para os férmions de Majorana são degeneradas. Para os TSCs extremamente curtos ($\varepsilon_M \rightarrow \infty$), o nível de energia ε_M para o orbital f está fora de ressonância com a energia da QI $\varepsilon_{\uparrow} = 0$, fazendo com que a QI e o TSC desacoplem-se. Assim, o canal de spin-up comporta-se como o correspondente do canal de spin-down, que está permanentemente desacoplado do TSC. Implicando assim, que a MIQ não pode ser observada para fios muito curtos.

A Fig. 4.3 resume nossas descobertas, exibindo mapas de cores para as DOSs eletrônicas e de Majorana, respectivamente, abrangendo ω e ε_M . Os painéis (a)-(c) descrevem o caso $S = 0$, que é caracterizado por $\text{DOS}(\uparrow)(0) = 1$ e $\text{DOS}(\uparrow)[\gamma_A](0) = \text{DOS}(\uparrow)[\gamma_B](0) = 1$. Isso corresponde ao regime trivial onde dois MZMs localizam em torno de energia zero e aparecem no sítio da QI.

Essa característica está nos picos de energia zero e aparece como linhas horizontais na representação dos painéis (a)-(c) para qualquer valor finito de ε_M . Como podemos ver, os picos secundários em (a) surgem de (c). Ao ativar a interação de Ising com $S = 3$ e $J = 5\Gamma$, os perfis espectrais das DOSs adquirem padrões distintos: os picos secundários obedecem aproximadamente à teoria padrão do momento angular para o desdobramento de Zeeman,

exibindo assim, $2S$ bandas. Nessa situação, a dependência linear do parâmetro de troca J está ausente. Além disso, as regiões centrais dos painéis (a)-(c) são convertidas em domínios delimitados por paredes em forma de cone como os encontrados em (d)-(f).

Embora essas paredes persistam até um limite em ε_M (não marcado na figura), uma interação entre o TSC e o termo de Ising governa a física do sistema e permite a possibilidade da existência da MIQ. Note que, para $\varepsilon_M > \Gamma$, uma estrutura central de múltiplos níveis $2S + 1$ finalmente é resolvida. Vale mencionar que para $\varepsilon_M = \Gamma$, os cortes de linha na Fig. 4.3 dados pelas linhas tracejadas verticais correspondem aos casos discutidos em detalhe na Fig. 4.2. Gostaríamos de mencionar que a escolha $\varepsilon_M = \Gamma$ corresponde a um limite extremo, apenas para melhor resolver nossas descobertas.

No entanto, enquanto ε_M permanece dentro dos domínios das paredes em forma de cone mencionados anteriormente, o efeito persiste. Nos painéis (e) e (f), notamos o surgimento do vale e das estruturas espectrais quase ressonante de MZM, respectivamente, ao aumentar ε_M . No entanto, muito acima do limite em ε_M , o espaçamento linear em J para o desdobramento de Zeeman é restaurado e essa situação é delimitada pelas linhas tracejadas horizontais marcadas.

Finalmente, os painéis (g)-(i) mostram a fusão da estrutura de múltiplos níveis no ponto especial $J = J_h = 1.335\Gamma$, levando ao surgimento do MIQ γ_B , enquanto o vale continua em γ_A . Portanto, dentro do domínio de paredes em forma de cone, o setor os férmions Majorana do tipo γ_B para a QI explicita um processo de interferência construtiva na energia zero, enquanto o correspondente em γ_A exibe um comportamento destrutivo. Nesse regime, a condutância $\mathcal{G}_{\text{LAR}}(0)$ é completamente suprimida e apenas $\mathcal{G}_{\text{ET}}(0)$ contribui para $\mathcal{G}_{\text{Total}}(0) = \frac{e^2}{2h}$ [Fig. 4.1(d)].

Capítulo 5

Conclusões

Através do estudo realizado, descobrimos que a fracionalização dos MZMs torna-se possível quando um spin inteiro S é acoplado a uma impureza quântica, a qual comporta-se como a nova borda do TSC finito em 1D. Um novo regime surge quando é aplicado um valor específico de acoplamento do tipo Ising, o que torna possível localizar um MZM fracionalizado no sistema. Apresentamos tal excitação como uma quasipartícula do tipo Majorana-Ising (MIQ).

Como resultado, apontamos o surgimento de um MZM que exibe o peso espectral pela metade e com um caráter ressonante. Em contraste, o outro modo de MZM na QI mostra o mesmo peso espectral do MZM ressonante, porém com um perfil antirressonante. Devido à localização do MIQ, metade do *quantum* de condutância dá-se devido à contribuição normal eletrônica, enquanto a reflexão de Andreev entre o QI e os terminais está totalmente ausente. Esse comportamento difere do observado nos TSCs infinitos, nos quais, um MZM localiza-se no sítio da QI com peso espectral máximo e com as condutâncias eletrônica e de Andreev contribuindo igualmente na ressonância em zero.

Portanto, nossa proposta aponta uma maneira de induzir, sob uma perspectiva mais realista do ponto de vista experimental, um estado quântico na borda de um TSC curto em 1D.

Capítulo 6

Publicações e perspectivas futuras

Destacamos aqui o artigo referente a este trabalho e os demais dos quais fiz parte, assim como os projetos para publicações futuras.

1) Publicações

- **Fractionalization of Majorana-Ising-type quasiparticle excitations.** J. E. Sanches, L. T. Lustosa, L. S. Ricco , I. A. Shelykh, M. de Souza , M. S. Figueira, and A. C. Seridonio, Phys. Rev. B 107, 155144 - Published 26 April 2023.
- **Analog of atomic collapse for adatoms on rhombohedral multilayer graphene.** W. C. Silva, J. E. Sanches, A. M. Freitas, L. T. Lustosa, M. de Souza, and A. C. Seridonio Phys. Rev. B 108, 205407 – Published 7 November 2023

2) Perspectivas futuras (Projetos em desenvolvimento)

- Análise das operações do tipo *braiding* obtidas por meio das funções de Green (em uma cadeia linear com quatro MZMs), considerando um acoplamento finito entre as componentes adjacentes de Majorana. É um sistema em que observamos a diferença de fase entre caminhos contra-propagantes escolhido como ponto de partida para as operações de *braiding*.
- Estudo do comportamento do modelo mínimo de Kitaev sob a influência de uma ponta spin-polarizada. Análise das densidades espectrais para o modelo mínimo e das quasipartículas de Majorana.

Capítulo 7

Impacto e relevância científico-social

A computação quântica emerge como uma fronteira tecnológica promissora, com o potencial de revolucionar a maneira como processamos informações. Ao optar por qubits em vez dos bits convencionais, ela desafia os limites da computação tradicional.

No entanto, a fragilidade dos qubits devido à decoerência quântica representa um desafio significativo. É nesse contexto que os férmions de Majorana surgem como uma solução revolucionária, oferecendo melhorias substanciais na estabilidade dos qubits e abrindo caminho para a construção de arquiteturas quânticas mais robustas.

Em resumo, o estudo dos férmions de Majorana pode ser essencial para o avanço da computação quântica, proporcionando uma base sólida para a criação de qubits mais estáveis e resistentes. A exploração dessas partículas não apenas supera os desafios enfrentados pela computação tradicional, mas também abre portas para a concretização de uma era em que sistemas quânticos avançados podem resolver eficientemente problemas complexos.

Todavia, a realização material desses férmions de Majorana é uma tarefa difícil, visto que na literatura esse é um objeto tratado, quase sempre, de forma idealizada, o que torna ainda mais difícil sua realização. Nesse cenário é que apresentamos uma proposta mais realista, que pode tornar possível a realização experimental deste candidato promissor ao qubit.

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Apêndice A

Apêndice

Cálculos realizados apara obtenção das DOSs

A.1 Obtenção das funções de Green

A função de Green, no domínio da energia, na notação de Zubarev é dada por $\omega^+ \langle\langle A; B \rangle\rangle = \langle\{A, B\}\rangle + \langle\langle [A, \mathcal{H}]; B \rangle\rangle$, onde o primeiro termo representa a média térmica e do segundo termo surge uma nova equação de Green. Calculando $\langle\langle d_\sigma; d_\sigma^\dagger \rangle\rangle$, temos

$$\omega^+ \langle\langle d_\sigma Y^{mm}; d_\sigma^\dagger \rangle\rangle = \langle\langle [d_\sigma Y^{mm}, d_\sigma^\dagger]_+ \rangle\rangle + \langle\langle [d_\sigma Y^{mm}, \mathcal{H}]; d_\sigma^\dagger \rangle\rangle. \quad (\text{A.1})$$

Do anticomutador temos

$$\begin{aligned} \langle\langle [d_\sigma Y^{mm}, d_\sigma^\dagger]_+ \rangle\rangle &= \langle\langle (d_\sigma Y^{mm} d_\sigma^\dagger + d_\sigma^\dagger d_\sigma Y^{mm}) \rangle\rangle \\ &= \langle\langle Y^{mm} (d_\sigma d_\sigma^\dagger + d_\sigma^\dagger d_\sigma) \rangle\rangle \\ &= \langle\langle Y^{mm} \delta_{\sigma\sigma} \rangle\rangle \\ \langle\langle [d_\sigma Y^{mm}, d_\sigma^\dagger]_+ \rangle\rangle &= \langle\langle Y^{mm} \rangle\rangle. \end{aligned} \quad (\text{A.2})$$

Do comutador, temos

$$\begin{aligned}
[d_\sigma Y^{mm}, \mathcal{H}] &= \left[d_\sigma Y^{mm}, \sum_{k\alpha\sigma'} \varepsilon_{k\alpha} c_{k\alpha\sigma'}^\dagger c_{k\alpha\sigma'} \right] + [d_\sigma Y^{mm}, \varepsilon_1 (n_\uparrow + n_\downarrow)] \\
&+ \left[d_\sigma Y^{mm}, \sum_{k\alpha\sigma'} \left(V_{k\alpha} c_{k\alpha\sigma'}^\dagger d_{\sigma'} + V_k^* d_{\sigma'}^\dagger c_{k\sigma'} \right) \right] \\
&+ \left[d_\sigma Y^{mm}, \frac{J}{2} \sum_m m n_\uparrow Y^{mm} \right] + \left[d_\sigma Y^{mm}, \left(-\frac{J}{2} \sum_m m n_\downarrow Y^{mm} \right) \right] \\
&+ [d_\sigma Y^{mm}, \mathcal{H}_{MZM}].
\end{aligned} \tag{A.3}$$

Resolvendo termo a termo o comutador, fica

$$\begin{aligned}
\left[d_\sigma Y^{mm}, \sum_{k\alpha\sigma'} \varepsilon_{k\alpha} c_{k\alpha\sigma'}^\dagger c_{k\alpha\sigma'} \right] &= \sum_{k\alpha\sigma'} \varepsilon_{k\alpha} [d_\sigma Y^{mm}, c_{k\alpha\sigma'}^\dagger c_{k\alpha\sigma'}] \\
&= \sum_{k\alpha\sigma'} \varepsilon_{k\alpha} \left(d_\sigma Y^{mm} c_{k\alpha\sigma'}^\dagger c_{k\alpha\sigma'} - c_{k\alpha\sigma'}^\dagger c_{k\alpha\sigma'} d_\sigma Y^{mm} \right) \\
&= \sum_{k\alpha\sigma'} \varepsilon_{k\alpha} \left(d_\sigma c_{k\alpha\sigma'}^\dagger c_{k\alpha\sigma'} Y^{mm} - c_{k\alpha\sigma'}^\dagger c_{k\alpha\sigma'} d_\sigma Y^{mm} \right) \\
&= \sum_{k\alpha\sigma'} \varepsilon_{k\alpha} \left(c_{k\alpha\sigma'}^\dagger c_{k\alpha\sigma'} d_\sigma Y^{mm} - c_{k\alpha\sigma'}^\dagger c_{k\alpha\sigma'} d_\sigma Y^{mm} \right) \\
\left[d_\sigma Y^{mm}, \sum_{k\alpha\sigma'} \varepsilon_{k\alpha} c_{k\alpha\sigma'}^\dagger c_{k\alpha\sigma'} \right] &= 0.
\end{aligned} \tag{A.4}$$

Para o segundo termo,

$$\begin{aligned}
[d_\sigma Y^{mm}, \varepsilon_1 (n_\uparrow + n_\downarrow)] &= \varepsilon_1 [d_\sigma Y^{mm}, (d_\uparrow^\dagger d_\uparrow + d_\downarrow^\dagger d_\downarrow)] \\
&= \varepsilon_1 \left[\left(d_\sigma Y^{mm} d_\uparrow^\dagger d_\uparrow - d_\uparrow^\dagger d_\uparrow d_\sigma Y^{mm} \right) + \left(d_\sigma Y^{mm} d_\downarrow^\dagger d_\downarrow - d_\downarrow^\dagger d_\downarrow d_\sigma Y^{mm} \right) \right] \\
&= \varepsilon_1 \left[\left(d_\sigma d_\uparrow^\dagger d_\uparrow Y^{mm} - d_\uparrow^\dagger d_\uparrow d_\sigma Y^{mm} \right) + \left(d_\sigma d_\downarrow^\dagger d_\downarrow Y^{mm} - d_\downarrow^\dagger d_\downarrow d_\sigma Y^{mm} \right) \right] \\
&= \varepsilon_1 \left[\left(\delta_{\sigma\uparrow} - d_\uparrow^\dagger d_\sigma \right) d_\uparrow Y^{mm} - d_\uparrow^\dagger d_\uparrow d_\sigma Y^{mm} \right] \\
&+ \varepsilon_1 \left[\left(\delta_{\sigma\downarrow} - d_\downarrow^\dagger d_\sigma \right) d_\downarrow Y^{mm} - d_\downarrow^\dagger d_\downarrow d_\sigma Y^{mm} \right] \\
&= \varepsilon_1 \left(\delta_{\sigma\uparrow} d_\uparrow Y^{mm} - d_\uparrow^\dagger d_\sigma d_\uparrow Y^{mm} - d_\uparrow^\dagger d_\uparrow d_\sigma Y^{mm} \right) \\
&+ \varepsilon_1 \left(\delta_{\sigma\downarrow} d_\downarrow Y^{mm} - d_\downarrow^\dagger d_\sigma d_\downarrow Y^{mm} - d_\downarrow^\dagger d_\downarrow d_\sigma Y^{mm} \right) \\
&= \varepsilon_1 \left(\delta_{\sigma\uparrow} d_\uparrow Y^{mm} + d_\uparrow^\dagger d_\uparrow d_\sigma Y^{mm} - d_\uparrow^\dagger d_\uparrow d_\sigma Y^{mm} \right) \\
&+ \varepsilon_1 \left(\delta_{\sigma\downarrow} d_\downarrow Y^{mm} + d_\downarrow^\dagger d_\downarrow d_\sigma Y^{mm} - d_\downarrow^\dagger d_\downarrow d_\sigma Y^{mm} \right) \\
[d_\sigma Y^{mm}, \varepsilon_1 (n_\uparrow + n_\downarrow)] &= \varepsilon_1 [\delta_{\sigma\uparrow} d_\uparrow Y^{mm} + \delta_{\sigma\downarrow} d_\downarrow Y^{mm}].
\end{aligned} \tag{A.5}$$

Para o terceiro termo,

$$\begin{aligned}
\left[d_\sigma Y^{mm}, \sum_{k\alpha\sigma'} \left(V_{k\alpha} c_{k\alpha\sigma'}^\dagger d_{\sigma'} + V_{k\alpha}^* d_{\sigma'}^\dagger c_{k\sigma'} \right) \right] &= \sum_{k\alpha\sigma'} \left[d_\sigma Y^{mm}, \left(V_{k\alpha} c_{k\alpha\sigma'}^\dagger d_{\sigma'} + V_{k\alpha}^* d_{\sigma'}^\dagger c_{k\sigma'} \right) \right] \\
&= \sum_{k\alpha\sigma'} [d_\sigma Y^{mm} V_{k\alpha} c_{k\alpha\sigma'}^\dagger d_{\sigma'} - c_{k\alpha\sigma'}^\dagger d_{\sigma'} d_\sigma Y^{mm} V] \\
&\quad + \sum_{k\alpha\sigma'} [d_\sigma Y^{mm} V_{k\alpha}^* d_{\sigma'}^\dagger c_{k\sigma'} - V_{k\alpha}^* d_{\sigma'}^\dagger c_{k\sigma'} d_\sigma Y^{mm}] \\
&= \sum_{k\alpha\sigma'} [V_{k\alpha} (d_\sigma Y^{mm} c_{k\alpha\sigma'}^\dagger d_{\sigma'} - c_{k\alpha\sigma'}^\dagger d_{\sigma'} d_\sigma Y^{mm})] \\
&\quad + \sum_{k\alpha\sigma'} [V_{k\alpha}^* (d_\sigma Y^{mm} d_{\sigma'}^\dagger c_{k\sigma'} - d_{\sigma'}^\dagger c_{k\sigma'} d_\sigma Y^{mm})] \\
&= \sum_{k\alpha\sigma'} [V_{k\alpha} (d_\sigma c_{k\alpha\sigma'}^\dagger d_{\sigma'} Y^{mm} - c_{k\alpha\sigma'}^\dagger d_{\sigma'} d_\sigma Y^{mm})] \\
&\quad + \sum_{k\alpha\sigma'} [V_{k\alpha}^* (d_\sigma d_{\sigma'}^\dagger c_{k\sigma'} Y^{mm} - d_{\sigma'}^\dagger c_{k\sigma'} d_\sigma Y^{mm})] \\
&= \sum_{k\alpha\sigma'} [V_{k\alpha} (-c_{k\alpha\sigma'}^\dagger d_\sigma d_{\sigma'} Y^{mm} - c_{k\alpha\sigma'}^\dagger d_{\sigma'} d_\sigma Y^{mm})] \\
&\quad + \sum_{k\alpha\sigma'} [V_{k\alpha}^* ((\delta_{\sigma\sigma'} - d_{\sigma'}^\dagger d_\sigma) c_{k\sigma'} Y^{mm} - d_{\sigma'}^\dagger c_{k\sigma'} d_\sigma Y^{mm})] \\
&= \sum_{k\alpha\sigma'} [V_{k\alpha} (c_{k\alpha\sigma'}^\dagger d_{\sigma'} d_\sigma Y^{mm} - c_{k\alpha\sigma'}^\dagger d_{\sigma'} d_\sigma Y^{mm})] \\
&\quad + \sum_{k\alpha\sigma'} [V_{k\alpha}^* (1 - d_{\sigma'}^\dagger d_\sigma) c_{k\sigma'} Y^{mm} - d_{\sigma'}^\dagger c_{k\sigma'} d_\sigma Y^{mm}] \\
&= \sum_{k\alpha\sigma'} [V_{k\alpha}^* (c_{k\sigma'} d_\sigma Y^{mm} - d_{\sigma'}^\dagger d_\sigma c_{k\sigma'} Y^{mm} - d_{\sigma'}^\dagger c_{k\sigma'} d_\sigma Y^{mm})] \\
&= \sum_{k\alpha\sigma'} [V_{k\alpha}^* (c_{k\sigma'} d_\sigma Y^{mm} + d_{\sigma'}^\dagger c_{k\sigma'} d_\sigma Y^{mm} - d_{\sigma'}^\dagger c_{k\sigma'} d_\sigma Y^{mm})] \\
\left[d_\sigma Y^{mm}, \sum_{k\alpha\sigma'} \left(V_{k\alpha} c_{k\alpha\sigma'}^\dagger d_{\sigma'} + V_{k\alpha}^* d_{\sigma'}^\dagger c_{k\sigma'} \right) \right] &= \sum_{k\alpha\sigma'} V_{k\alpha}^* c_{k\alpha\sigma'} d_\sigma Y^{mm}. \tag{A.6}
\end{aligned}$$

Para o quarto termo,

$$\begin{aligned}
[d_\sigma Y^{mm}, \frac{J}{2} \sum_{m'} m' n_\uparrow Y^{m'm'}] &= \frac{J}{2} \sum_{m'} m' [d_\sigma Y^{mm}, d_\uparrow^\dagger d_\uparrow Y^{m'm'}] \\
&= \frac{J}{2} \sum_{m'} m' [d_\sigma Y^{mm} d_\uparrow^\dagger d_\uparrow Y^{m'm'}] \\
&\quad - \frac{J}{2} \sum_{m'} m' [d_\uparrow^\dagger d_\uparrow Y^{m'm'} d_\sigma Y^{mm}] \\
&= \frac{J}{2} \sum_{m'} m' [d_\sigma d_\uparrow^\dagger d_\uparrow Y^{mm} Y^{m'm'}] \\
&\quad - \frac{J}{2} \sum_{m'} m' [d_\uparrow^\dagger d_\uparrow d_\sigma Y^{m'm'} Y^{mm}]. \tag{A.7}
\end{aligned}$$

Utilizando a regra

$$Y^{ab} Y^{cd} = \delta_{bc} Y^{ad}. \tag{A.8}$$

Então a Eq. (A.7), fica

$$\begin{aligned}
\left[d_\sigma Y^{mm}, \frac{J}{2} \sum_{m'} m' n_\uparrow Y^{m'm'} \right] &= \frac{J}{2} \sum_{m'} m' \left[d_\sigma d_\uparrow^\dagger d_\uparrow Y^{mm} Y^{m'm'} - d_\uparrow^\dagger d_\uparrow d_\sigma Y^{m'm'} Y^{mm} \right] \\
&= \frac{J}{2} \sum_{m'} m' \left[d_\sigma d_\uparrow^\dagger d_\uparrow (\delta_{mm'} Y^{mm'}) - d_\uparrow^\dagger d_\uparrow d_\sigma (\delta_{m'm} Y^{m'm}) \right] \\
&= \frac{J}{2} \sum_{m'} m' \left[(\delta_{\sigma\uparrow} - d_\uparrow^\dagger d_\sigma) d_\uparrow (\delta_{mm'} Y^{mm'}) - d_\uparrow^\dagger d_\uparrow d_\sigma (\delta_{m'm} Y^{m'm}) \right] \\
&= \frac{J}{2} \sum_{m'} m' \left[(\delta_{\sigma\uparrow} d_\uparrow (\delta_{mm'} Y^{mm'}) - d_\uparrow^\dagger d_\sigma d_\uparrow (\delta_{mm'} Y^{mm'})) \right. \\
&\quad \left. - \frac{J}{2} \sum_{m'} m' [(d_\uparrow^\dagger d_\uparrow d_\sigma (\delta_{m'm} Y^{m'm}))] \right] \\
&= \frac{J}{2} \sum_{m'} m' \left[(\delta_{\sigma\uparrow} d_\uparrow (\delta_{mm'} Y^{mm'}) + d_\uparrow^\dagger d_\uparrow d_\sigma (\delta_{mm'} Y^{mm'})) \right. \\
&\quad \left. - \frac{J}{2} \sum_{m'} m' [(d_\uparrow^\dagger d_\uparrow d_\sigma (\delta_{m'm} Y^{m'm}))] \right] \\
&= \frac{J}{2} \left[(\delta_{\sigma\uparrow} d_\uparrow (\sum_{m'} m' \delta_{mm'} Y^{mm'}) + d_\uparrow^\dagger d_\uparrow d_\sigma (\sum_{m'} m' \delta_{mm'} Y^{mm'})) \right. \\
&\quad \left. - \frac{J}{2} d_\uparrow^\dagger d_\uparrow d_\sigma (\sum_{m'} m' \delta_{m'm} Y^{m'm}) \right] \\
&= \frac{J}{2} \left[(\delta_{\sigma\uparrow} d_\uparrow (m' Y^{mm'}) + d_\uparrow^\dagger d_\uparrow d_\sigma (m' Y^{mm'}) - d_\uparrow^\dagger d_\uparrow d_\sigma (m' Y^{m'm})) \right] \\
&= \frac{J}{2} \left[(\delta_{\sigma\uparrow} d_\uparrow (m Y^{mm}) + d_\uparrow^\dagger d_\uparrow d_\sigma (m Y^{mm}) - d_\uparrow^\dagger d_\uparrow d_\sigma (m Y^{mm})) \right] \\
\left[d_\sigma Y^{mm}, \frac{J}{2} \sum_{m'} m' n_\uparrow Y^{m'm'} \right] &= \frac{J}{2} \delta_{\sigma\uparrow} d_\uparrow (m Y^{mm}). \tag{A.9}
\end{aligned}$$

Para o quinto termo,

$$\begin{aligned}
\left[d_\sigma Y^{mm}, \frac{J}{2} \sum_{m'} m' n_\downarrow Y^{m'm'} \right] &= -\frac{J}{2} \sum_{m'} m' \left[d_\sigma Y^{mm}, d_\downarrow^\dagger d_\downarrow Y^{m'm'} \right] \\
&= -\frac{J}{2} \sum_{m'} m' \left[d_\sigma Y^{mm} d_\downarrow^\dagger d_\downarrow Y^{m'm'} - d_\downarrow^\dagger d_\downarrow Y^{m'm'} d_\sigma Y^{mm} \right] \\
\left[d_\sigma Y^{mm}, \frac{J}{2} \sum_{m'} m' n_\downarrow Y^{m'm'} \right] &= -\frac{J}{2} \sum_{m'} m' \left[d_\sigma d_\downarrow^\dagger d_\downarrow Y^{mm} Y^{m'm'} - d_\downarrow^\dagger d_\downarrow d_\sigma Y^{m'm'} Y^{mm} \right] \tag{A.10}
\end{aligned}$$

A Eq. (A.10), fica

$$\begin{aligned}
\left[d_\sigma Y^{mm}, \frac{J}{2} \sum_{m'} m' n_\downarrow Y^{m'm'} \right] &= -\frac{J}{2} \sum_{m'} m' \left[d_\sigma d_\downarrow^\dagger d_\downarrow Y^{mm} Y^{m'm'} - d_\downarrow^\dagger d_\downarrow d_\sigma Y^{m'm'} Y^{mm} \right] \\
&= -\frac{J}{2} \sum_{m'} m' \left[d_\sigma d_\downarrow^\dagger d_\downarrow \left(\delta_{mm'} Y^{mm'} \right) - d_\downarrow^\dagger d_\downarrow d_\sigma \left(\delta_{m'm} Y^{m'm} \right) \right] \\
&= -\frac{J}{2} \sum_{m'} m' \left[\left(\delta_{\sigma\downarrow} - d_\downarrow^\dagger d_\sigma \right) d_\downarrow \left(\delta_{mm'} Y^{mm'} \right) - d_\downarrow^\dagger d_\downarrow d_\sigma \left(\delta_{m'm} Y^{m'm} \right) \right] \\
&= -\frac{J}{2} \sum_{m'} m' \left[\delta_{\sigma\downarrow} d_\downarrow \left(\delta_{mm'} Y^{mm'} \right) - d_\downarrow^\dagger d_\sigma d_\downarrow \left(\delta_{mm'} Y^{mm'} \right) \right] \\
&+ \frac{J}{2} \sum_{m'} m' \left[d_\downarrow^\dagger d_\downarrow d_\sigma \left(\delta_{m'm} Y^{m'm} \right) \right] \\
&= -\frac{J}{2} \sum_{m'} m' \left[\delta_{\sigma\downarrow} d_\downarrow \left(\delta_{mm'} Y^{mm'} \right) + d_\downarrow^\dagger d_\downarrow d_\sigma \left(\delta_{mm'} Y^{mm'} \right) \right] \\
&+ \frac{J}{2} \sum_{m'} m' \left[d_\downarrow^\dagger d_\downarrow d_\sigma \left(\delta_{m'm} Y^{m'm} \right) \right] \\
&= \frac{-J}{2} \left[\delta_{\sigma\downarrow} d_\downarrow \left(\sum_{m'} m' \delta_{mm'} Y^{mm'} \right) + d_\downarrow^\dagger d_\downarrow d_\sigma \left(\sum_{m'} m' \delta_{mm'} Y^{mm'} \right) \right] \\
&+ \frac{J}{2} d_\downarrow^\dagger d_\downarrow d_\sigma \left(\sum_{m'} m' \delta_{m'm} Y^{m'm} \right) \\
&= \frac{-J}{2} \left[\delta_{\sigma\downarrow} d_\downarrow \left(m' Y^{mm'} \right) + d_\downarrow^\dagger d_\downarrow d_\sigma \left(m' Y^{mm'} \right) - d_\downarrow^\dagger d_\downarrow d_\sigma \left(m' Y^{m'm} \right) \right] \\
&= \frac{-J}{2} \left[\delta_{\sigma\downarrow} d_\downarrow \left(m Y^{mm} \right) + d_\downarrow^\dagger d_\downarrow d_\sigma \left(m Y^{mm} \right) - d_\downarrow^\dagger d_\downarrow d_\sigma \left(m Y^{mm} \right) \right] \\
\left[d_\sigma Y^{mm}, \frac{J}{2} \sum_{m'} m' n_\downarrow Y^{m'm'} \right] &= \frac{-J}{2} \delta_{\sigma\downarrow} d_\downarrow \left(m Y^{mm} \right). \tag{A.11}
\end{aligned}$$

Para o último Termo,

$$\begin{aligned}
[d_\sigma Y^{mm}, \mathcal{H}_{MZM}] &= \left[d_\sigma Y^{mm}, (\varepsilon_M f^\dagger f + t d_\uparrow f^\dagger + \Delta f^\dagger d_\uparrow^\dagger \right. \\
&\quad \left. + t f d_\uparrow^\dagger + \Delta d_\uparrow f - \frac{\varepsilon_M}{2}) \right] \\
[d_\sigma Y^{mm}, \mathcal{H}_{MZM}] &= [d_\sigma Y^{mm}, \varepsilon_M f^\dagger f] + [d_\sigma Y^{mm}, t d_\uparrow f^\dagger] \\
&\quad + [d_\sigma Y^{mm}, \Delta f^\dagger d_\uparrow^\dagger] + [d_\sigma Y^{mm}, t f d_\uparrow^\dagger] \\
&\quad + [d_\sigma Y^{mm}, \Delta d_\uparrow f] - [d_\sigma Y^{mm}, \frac{\varepsilon_M}{2}]. \tag{A.12}
\end{aligned}$$

Resolvendo termo a termo a Eq. (A.12), temos

Para o primeiro termo,

$$\begin{aligned}
[d_\sigma Y^{mm}, \varepsilon_M f^\dagger f] &= \varepsilon_M [d_\sigma Y^{mm} f^\dagger f - f^\dagger f d_\sigma Y^{mm}] \\
&= \varepsilon_M [d_\sigma f^\dagger f Y^{mm} - f^\dagger f d_\sigma Y^{mm}] \\
&= \varepsilon_M [-f^\dagger d_\sigma f Y^{mm} - f^\dagger f d_\sigma Y^{mm}] \\
&= \varepsilon_M [f^\dagger f d_\sigma Y^{mm} - f^\dagger f d_\sigma Y^{mm}] \\
[d_\sigma Y^{mm}, \varepsilon_M f^\dagger f] &= 0.
\end{aligned} \tag{A.13}$$

Para o segundo termo,

$$\begin{aligned}
[d_\sigma Y^{mm}, t d_\uparrow f^\dagger] &= t [d_\sigma Y^{mm} d_\uparrow f^\dagger - d_\uparrow f^\dagger d_\sigma Y^{mm}] \\
&= t [d_\sigma d_\uparrow f^\dagger Y^{mm} - d_\uparrow f^\dagger d_\sigma Y^{mm}] \\
&= t [d_\sigma d_\uparrow f^\dagger Y^{mm} - d_\uparrow f^\dagger d_\sigma Y^{mm}] \\
&= t [-d_\uparrow d_\sigma f^\dagger Y^{mm} - d_\uparrow f^\dagger d_\sigma Y^{mm}] \\
&= t [d_\uparrow f^\dagger d_\sigma Y^{mm} - d_\uparrow f^\dagger d_\sigma Y^{mm}] \\
[d_\sigma Y^{mm}, t d_\uparrow f^\dagger] &= 0.
\end{aligned} \tag{A.14}$$

Para o terceiro termo,

$$\begin{aligned}
[d_\sigma Y^{mm}, \Delta f^\dagger d_\uparrow^\dagger] &= \Delta [d_\sigma Y^{mm} f^\dagger d_\uparrow^\dagger - f^\dagger d_\uparrow^\dagger d_\sigma Y^{mm}] \\
&= \Delta [d_\sigma f^\dagger d_\uparrow^\dagger Y^{mm} - f^\dagger d_\uparrow^\dagger d_\sigma Y^{mm}] \\
&= \Delta [-f^\dagger d_\sigma d_\uparrow^\dagger Y^{mm} - f^\dagger d_\uparrow^\dagger d_\sigma Y^{mm}] \\
&= \Delta [-f^\dagger (\delta_{\sigma\uparrow} - d_\uparrow^\dagger d_\sigma) Y^{mm} - f^\dagger d_\uparrow^\dagger d_\sigma Y^{mm}] \\
&= \Delta [-f^\dagger Y^{mm} \delta_{\sigma\uparrow} + f^\dagger d_\uparrow^\dagger d_\sigma Y^{mm} - f^\dagger d_\uparrow^\dagger d_\sigma Y^{mm}] \\
[d_\sigma Y^{mm}, \Delta f^\dagger d_\uparrow^\dagger] &= -\Delta f^\dagger Y^{mm} \delta_{\sigma\uparrow}.
\end{aligned} \tag{A.15}$$

Para o quarto termo,

$$\begin{aligned}
[d_\sigma Y^{mm}, t f d_\uparrow^\dagger] &= t [d_\sigma Y^{mm} f d_\uparrow^\dagger - f d_\uparrow^\dagger d_\sigma Y^{mm}] \\
&= t [d_\sigma f d_\uparrow^\dagger Y^{mm} - f d_\uparrow^\dagger d_\sigma Y^{mm}] \\
&= t [-f d_\sigma d_\uparrow^\dagger Y^{mm} - f d_\uparrow^\dagger d_\sigma Y^{mm}] \\
&= t [-f (\delta_{\sigma\uparrow} - d_\uparrow^\dagger d_\sigma) Y^{mm} - f d_\uparrow^\dagger d_\sigma Y^{mm}] \\
&= t [-f Y^{mm} \delta_{\sigma\uparrow} + f d_\uparrow^\dagger d_\sigma Y^{mm} - f d_\uparrow^\dagger d_\sigma Y^{mm}] \\
[d_\sigma Y^{mm}, t f d_\uparrow^\dagger] &= -t f Y^{mm} \delta_{\sigma\uparrow}.
\end{aligned} \tag{A.16}$$

Para o quinto termo,

$$\begin{aligned}
[d_\sigma Y^{mm}, \Delta d_\uparrow f] &= \Delta [d_\sigma Y^{mm} d_\uparrow f - d_\uparrow f d_\sigma Y^{mm}] \\
&= \Delta [d_\sigma d_\uparrow f Y^{mm} - d_\uparrow f d_\sigma Y^{mm}] \\
&= \Delta [-d_\uparrow d_\sigma f Y^{mm} - d_\uparrow f d_\sigma Y^{mm}] \\
&= \Delta [d_\uparrow f d_\sigma Y^{mm} - d_\uparrow f d_\sigma Y^{mm}] \\
[d_\sigma Y^{mm}, \Delta d_\uparrow f] &= 0.
\end{aligned} \tag{A.17}$$

Substituindo os valores encontrados na Eq. (A.1), temos

$$\begin{aligned}
\omega^+ \langle \langle d_\sigma Y^{mm}; d_\sigma^\dagger \rangle \rangle &= \langle Y^{mm} \rangle + \left\langle \left\langle \sum_{k\alpha\sigma'} V_{k\alpha}^* c_{k\alpha\sigma'} Y^{mm}; d_\sigma^\dagger \right\rangle \right\rangle \\
&+ \langle \langle \varepsilon_1 \delta_{\sigma\uparrow} d_\uparrow Y^{mm}; d_\sigma^\dagger \rangle \rangle + \langle \langle \varepsilon_1 \delta_{\sigma\downarrow} d_\downarrow Y^{mm}; d_\sigma^\dagger \rangle \rangle \\
&+ \left\langle \left\langle \frac{J}{2} \delta_{\sigma\uparrow} d_\uparrow m Y^{mm}; d_\sigma^\dagger \right\rangle \right\rangle + \left\langle \left\langle -\frac{J}{2} \delta_{\sigma\downarrow} d_\downarrow m Y^{mm}; d_\sigma^\dagger \right\rangle \right\rangle \\
&+ \langle \langle -\Delta f^\dagger Y^{mm} \delta_{\sigma\uparrow}; d_\sigma^\dagger \rangle \rangle + \langle \langle -t f Y^{mm} \delta_{\sigma\uparrow}; d_\sigma^\dagger \rangle \rangle.
\end{aligned} \tag{A.18}$$

Então, a Eq. (A.18), fica

$$\begin{aligned}
\omega^+ \langle \langle d_\sigma Y^{mm}; d_\sigma^\dagger \rangle \rangle &= \langle Y^{mm} \rangle + \sum_{k\alpha\sigma'} V_{k\alpha}^* \langle \langle c_{k\alpha\sigma'} Y^{mm}; d_\sigma^\dagger \rangle \rangle \\
&+ \varepsilon_1 \delta_{\sigma\uparrow} \langle \langle d_\uparrow Y^{mm}; d_\sigma^\dagger \rangle \rangle + \varepsilon_1 \delta_{\sigma\downarrow} \langle \langle d_\downarrow Y^{mm}; d_\sigma^\dagger \rangle \rangle \\
&+ \frac{J}{2} \delta_{\sigma\uparrow} \langle \langle d_\uparrow m Y^{mm}; d_\sigma^\dagger \rangle \rangle - \frac{J}{2} \delta_{\sigma\downarrow} \langle \langle d_\downarrow m Y^{mm}; d_\sigma^\dagger \rangle \rangle \\
&+ -\Delta \delta_{\sigma\uparrow} \langle \langle f^\dagger Y^{mm}; d_\sigma^\dagger \rangle \rangle - t \delta_{\sigma\uparrow} \langle \langle f Y^{mm}; d_\sigma^\dagger \rangle \rangle.
\end{aligned} \tag{A.19}$$

Quando analisamos a Eq. (A.19) para o spin-up ($\sigma = \uparrow$) a equação fica

$$\begin{aligned}
\omega^+ \left\langle \left\langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \right\rangle \right\rangle &= \langle Y^{mm} \rangle + \sum_{k\alpha\sigma'} V_{k\alpha}^* \left\langle \left\langle c_{k\alpha\sigma'} Y^{mm}; d_{\uparrow}^{\dagger} \right\rangle \right\rangle \\
&+ \varepsilon_1 \delta_{\uparrow\uparrow} \left\langle \left\langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \right\rangle \right\rangle + \frac{Jm}{2} \delta_{\uparrow\uparrow} \left\langle \left\langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \right\rangle \right\rangle \\
&- \Delta \delta_{\uparrow\uparrow} \left\langle \left\langle f^{\dagger} Y^{mm}; d_{\uparrow}^{\dagger} \right\rangle \right\rangle - t \delta_{\uparrow\uparrow} \left\langle \left\langle f Y^{mm}; d_{\uparrow}^{\dagger} \right\rangle \right\rangle. \quad (A.20)
\end{aligned}$$

$$\begin{aligned}
\omega^+ \left\langle \left\langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \right\rangle \right\rangle &= \langle Y^{mm} \rangle + \sum_{k\alpha\sigma'} V_{k\alpha}^* \left\langle \left\langle c_{k\alpha\sigma'} Y^{mm}; d_{\uparrow}^{\dagger} \right\rangle \right\rangle \\
&+ \varepsilon_1 \left\langle \left\langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \right\rangle \right\rangle + \frac{Jm}{2} \left\langle \left\langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \right\rangle \right\rangle \\
&- \Delta \left\langle \left\langle f^{\dagger} Y^{mm}; d_{\uparrow}^{\dagger} \right\rangle \right\rangle - t \left\langle \left\langle f Y^{mm}; d_{\uparrow}^{\dagger} \right\rangle \right\rangle. \quad (A.21)
\end{aligned}$$

Isolando os termos que possui $\left\langle \left\langle d_{\sigma} Y^{mm}; d_{\uparrow}^{\dagger} \right\rangle \right\rangle$, temos

$$\begin{aligned}
\omega^+ \left\langle \left\langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \right\rangle \right\rangle - \varepsilon_1 \left\langle \left\langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \right\rangle \right\rangle - \frac{Jm}{2} \left\langle \left\langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \right\rangle \right\rangle &= \langle Y^{mm} \rangle \\
&+ \sum_{k\alpha\sigma'} V_{k\alpha}^* \left\langle \left\langle c_{k\alpha\sigma'} Y^{mm}; d_{\uparrow}^{\dagger} \right\rangle \right\rangle \\
&- \Delta \left\langle \left\langle f^{\dagger} Y^{mm}; d_{\uparrow}^{\dagger} \right\rangle \right\rangle \\
&- t \left\langle \left\langle f Y^{mm}; d_{\uparrow}^{\dagger} \right\rangle \right\rangle. \quad (A.22)
\end{aligned}$$

Reescrevendo, temos

$$\begin{aligned}
\left(\omega^+ - \varepsilon_1 - \frac{Jm}{2} \right) \left\langle \left\langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \right\rangle \right\rangle &= \langle Y^{mm} \rangle + \sum_{k\alpha\sigma'} V_{k\alpha}^* \left\langle \left\langle c_{k\alpha\sigma'} Y^{mm}; d_{\uparrow}^{\dagger} \right\rangle \right\rangle \\
&- \Delta \left\langle \left\langle f^{\dagger} Y^{mm}; d_{\uparrow}^{\dagger} \right\rangle \right\rangle - t \left\langle \left\langle f Y^{mm}; d_{\uparrow}^{\dagger} \right\rangle \right\rangle. \quad (A.23)
\end{aligned}$$

Agora é necessário calcular as Funções de Green do majorana $\left\langle \left\langle f^{\dagger} Y^{mm}; d_{\sigma}^{\dagger} \right\rangle \right\rangle$ e $\left\langle \left\langle f Y^{mm}; d_{\sigma}^{\dagger} \right\rangle \right\rangle$,

$$\omega^+ \left\langle \left\langle f^{\dagger} Y^{mm}; d_{\sigma}^{\dagger} \right\rangle \right\rangle = \left\langle \left[f^{\dagger} Y^{mm}, d_{\sigma}^{\dagger} \right]_{+} \right\rangle + \left\langle \left[f^{\dagger} Y^{mm}, \mathcal{H} \right]; d_{\sigma}^{\dagger} \right\rangle. \quad (A.24)$$

Para o primeiro termo, temos

$$\begin{aligned}
[f^\dagger Y^{mm}; d_\sigma^\dagger]_+ &= Y^{mm} [f^\dagger d_\sigma^\dagger + d_\sigma^\dagger f^\dagger] \\
&= Y^{mm} [-d_\sigma^\dagger f^\dagger + d_\sigma^\dagger f^\dagger] \\
[f^\dagger Y^{mm}; d_\sigma^\dagger]_+ &= 0.
\end{aligned} \tag{A.25}$$

Para o segundo termo, vamos primeiro calcular $[f^\dagger Y^{mm}, \mathcal{H}]$

$$\begin{aligned}
[f^\dagger Y^{mm}, \mathcal{H}] &= \left[f^\dagger Y^{mm}, \sum_{k\alpha\sigma'} \varepsilon_{k\alpha} c_{k\alpha\sigma'}^\dagger c_{k\alpha\sigma'} \right] + [f^\dagger Y^{mm}, \varepsilon_1 (n_\uparrow + n_\downarrow)] \\
&+ \left[f^\dagger Y^{mm}, \sum_{k\alpha\sigma'} \left(V_{k\alpha} c_{k\alpha\sigma'}^\dagger d_{\sigma'} + V_k^* d_{\sigma'}^\dagger c_{k\sigma'} \right) \right] \\
&+ \left[f^\dagger Y^{mm}, \frac{J}{2} \sum_m m n_\uparrow Y^{mm} \right] + \left[f^\dagger Y^{mm}, \left(-\frac{J}{2} \sum_m m n_\downarrow Y^{mm} \right) \right] \\
&+ [f^\dagger Y^{mm}, \mathcal{H}_{MZM}].
\end{aligned} \tag{A.26}$$

Calculando termo a termo a Eq. (A.26)

$$\begin{aligned}
\left[f^\dagger Y^{mm}, \sum_{k\alpha\sigma'} \varepsilon_{k\alpha} c_{k\alpha\sigma'}^\dagger c_{k\alpha\sigma'} \right] &= \sum_{k\alpha\sigma'} \varepsilon_{k\alpha} \left(f^\dagger Y^{mm} c_{k\alpha\sigma'}^\dagger c_{k\alpha\sigma'} - c_{k\alpha\sigma'}^\dagger c_{k\alpha\sigma'} f^\dagger Y^{mm} \right) \\
&= \sum_{k\alpha\sigma'} \varepsilon_{k\alpha} \left(f^\dagger c_{k\alpha\sigma'}^\dagger c_{k\alpha\sigma'} Y^{mm} - c_{k\alpha\sigma'}^\dagger c_{k\alpha\sigma'} f^\dagger Y^{mm} \right) \\
&= \sum_{k\alpha\sigma'} \varepsilon_{k\alpha} \left(-c_{k\alpha\sigma'}^\dagger f^\dagger c_{k\alpha\sigma'} Y^{mm} - c_{k\alpha\sigma'}^\dagger c_{k\alpha\sigma'} f^\dagger Y^{mm} \right) \\
&= \sum_{k\alpha\sigma'} \varepsilon_{k\alpha} \left(c_{k\alpha\sigma'}^\dagger c_{k\alpha\sigma'} f^\dagger Y^{mm} - c_{k\alpha\sigma'}^\dagger c_{k\alpha\sigma'} f^\dagger Y^{mm} \right) \\
\left[f^\dagger Y^{mm}, \sum_{k\alpha\sigma'} \varepsilon_{k\alpha} c_{k\alpha\sigma'}^\dagger c_{k\alpha\sigma'} \right] &= 0,
\end{aligned} \tag{A.27}$$

$$\begin{aligned}
[f^\dagger Y^{mm}, \varepsilon_1 (n_\uparrow + n_\downarrow)] &= \varepsilon_1 [f^\dagger Y^{mm}, (d_\uparrow^\dagger d_\uparrow + d_\downarrow^\dagger d_\downarrow)] \\
&= \varepsilon_1 \left[\left(f^\dagger Y^{mm} d_\uparrow^\dagger d_\uparrow - d_\uparrow^\dagger d_\uparrow f^\dagger Y^{mm} \right) + \left(f^\dagger Y^{mm} d_\downarrow^\dagger d_\downarrow - d_\downarrow^\dagger d_\downarrow f^\dagger Y^{mm} \right) \right] \\
&= \varepsilon_1 \left[\left(f^\dagger d_\uparrow^\dagger d_\uparrow Y^{mm} - d_\uparrow^\dagger d_\uparrow f^\dagger Y^{mm} \right) + \left(f^\dagger d_\downarrow^\dagger d_\downarrow Y^{mm} - d_\downarrow^\dagger d_\downarrow f^\dagger Y^{mm} \right) \right] \\
&= \varepsilon_1 \left[\left(-d_\uparrow^\dagger f^\dagger d_\uparrow Y^{mm} - d_\uparrow^\dagger d_\uparrow f^\dagger Y^{mm} \right) + \left(-d_\downarrow^\dagger f^\dagger d_\downarrow Y^{mm} - d_\downarrow^\dagger d_\downarrow f^\dagger Y^{mm} \right) \right] \\
&= \varepsilon_1 \left[\left(d_\uparrow^\dagger d_\uparrow f^\dagger Y^{mm} - d_\uparrow^\dagger d_\uparrow f^\dagger Y^{mm} \right) + \left(d_\downarrow^\dagger d_\downarrow f^\dagger Y^{mm} - d_\downarrow^\dagger d_\downarrow f^\dagger Y^{mm} \right) \right] \\
[f^\dagger Y^{mm}, \varepsilon_1 (n_\uparrow + n_\downarrow)] &= 0.
\end{aligned} \tag{A.28}$$

É possível perceber que sempre estivermos trabalhando com operadores diferentes, seu anti-comutador será igual a zero. Por isso, a partir de agora, será omitido a resolução e admitiremos que seu valor é nulo diretamente. Então

$$\left[f^\dagger Y^{mm}, \sum_{k\alpha\sigma'} \left(V_{k\alpha} c_{k\alpha\sigma'}^\dagger d_{\sigma'} + V_{k\alpha}^* d_{\alpha\sigma'}^\dagger c_{k\sigma'} \right) \right] = 0; \tag{A.29}$$

$$\left[f^\dagger Y^{mm}, \frac{J}{2} \sum_m m n_\uparrow Y^{mm} \right] = 0; \tag{A.30}$$

$$\left[f^\dagger Y^{mm}, \left(-\frac{J}{2} \sum_m m n_\downarrow Y^{mm} \right) \right] = 0. \tag{A.31}$$

Resolvendo o último termo da Eq. (A.26)

$$\begin{aligned}
[f^\dagger Y^{mm}, \mathcal{H}_{MZM}] &= [f^\dagger Y^{mm}, (\varepsilon_M f^\dagger f + t d_\uparrow f^\dagger + \Delta f^\dagger d_\uparrow^\dagger + t f d_\uparrow^\dagger + \Delta d_\uparrow f)] \\
[f^\dagger Y^{mm}, \mathcal{H}_{MZM}] &= [f^\dagger Y^{mm}, \varepsilon_M f^\dagger f] + [f^\dagger Y^{mm}, t d_\uparrow f^\dagger] + [f^\dagger Y^{mm}, \Delta f^\dagger d_\uparrow^\dagger] \\
&+ [f^\dagger Y^{mm}, t f d_\uparrow^\dagger] + [f^\dagger Y^{mm}, \Delta d_\uparrow f].
\end{aligned} \tag{A.32}$$

Resolvendo termo a termo a Eq. (A.32)

$$\begin{aligned}
\left[f^\dagger Y^{mm}, \varepsilon_M f^{\dagger'} f \right] &= \varepsilon_M \left[f^\dagger Y^{mm}, f^{\dagger'} f \right] \\
&= \varepsilon_M \left(f^\dagger Y^{mm} f^{\dagger'} f - f^{\dagger'} f f^\dagger Y^{mm} \right) \\
&= \varepsilon_M \left(f^\dagger f^{\dagger'} f Y^{mm} - f^{\dagger'} f f^\dagger Y^{mm} \right) \\
&= \varepsilon_M \left(-f^{\dagger'} f^\dagger f Y^{mm} - f^{\dagger'} f f^\dagger Y^{mm} \right) \\
&= \varepsilon_M \left[-f^{\dagger'} (1 - f f^\dagger) Y^{mm} - f^{\dagger'} f f^\dagger Y^{mm} \right] \\
&= \varepsilon_M \left[-f^{\dagger'} Y^{mm} + f^{\dagger'} f f^\dagger Y^{mm} - f^{\dagger'} f f^\dagger Y^{mm} \right] \\
&= -\varepsilon_M f^{\dagger'} Y^{mm} \\
\left[f^\dagger Y^{mm}, \varepsilon_M f^{\dagger'} f \right] &= -\varepsilon_M f^{\dagger'} Y^{mm}; \tag{A.33}
\end{aligned}$$

$$\begin{aligned}
\left[f^\dagger Y^{mm}, t d_\uparrow f^{\dagger'} \right] &= t \left[f^\dagger Y^{mm} d_\uparrow f^{\dagger'} - d_\uparrow f^{\dagger'} f^\dagger Y^{mm} \right] \\
&= t \left[f^\dagger d_\uparrow f^{\dagger'} Y^{mm} - d_\uparrow f^{\dagger'} f^\dagger Y^{mm} \right] \\
&= t \left[-d_\uparrow f^\dagger f^{\dagger'} Y^{mm} - d_\uparrow f^{\dagger'} f^\dagger Y^{mm} \right] \\
&= t \left[d_\uparrow f^{\dagger'} f^\dagger Y^{mm} - d_\uparrow f^{\dagger'} f^\dagger Y^{mm} \right] \\
\left[f^\dagger Y^{mm}, t d_\uparrow f^{\dagger'} \right] &= 0; \tag{A.34}
\end{aligned}$$

$$\begin{aligned}
\left[f^\dagger Y^{mm}, \Delta f^{\dagger'} d_\uparrow^\dagger \right] &= \Delta \left[f^\dagger Y^{mm} f^{\dagger'} d_\uparrow^\dagger - f^{\dagger'} d_\uparrow^\dagger f^\dagger Y^{mm} \right] \\
&= \Delta \left[f^\dagger Y^{mm} f^{\dagger'} d_\uparrow^\dagger - f^{\dagger'} d_\uparrow^\dagger f^\dagger Y^{mm} \right] \\
&= \Delta \left[f^\dagger f^{\dagger'} d_\uparrow^\dagger Y^{mm} - f^{\dagger'} d_\uparrow^\dagger f^\dagger Y^{mm} \right] \\
&= \Delta \left[-f^{\dagger'} f^\dagger d_\uparrow^\dagger Y^{mm} - f^{\dagger'} d_\uparrow^\dagger f^\dagger Y^{mm} \right] \\
&= \Delta \left[f^{\dagger'} d_\uparrow^\dagger f^\dagger Y^{mm} - f^{\dagger'} d_\uparrow^\dagger f^\dagger Y^{mm} \right] \\
\left[f^\dagger Y^{mm}, \Delta f^{\dagger'} d_\uparrow^\dagger \right] &= 0; \tag{A.35}
\end{aligned}$$

$$\begin{aligned}
[f^\dagger Y^{mm}, \Delta t f d_\uparrow^\dagger] &= t [f^\dagger Y^{mm} f d_\uparrow^\dagger - f d_\uparrow^\dagger f^\dagger Y^{mm}] \\
&= t [f^\dagger f d_\uparrow^\dagger Y^{mm} - f d_\uparrow^\dagger f^\dagger Y^{mm}] \\
&= t [f^\dagger f d_\uparrow^\dagger Y^{mm} - f d_\uparrow^\dagger f^\dagger Y^{mm}] \\
&= t [(1 - f f^\dagger) d_\uparrow^\dagger Y^{mm} - f d_\uparrow^\dagger f^\dagger Y^{mm}] \\
&= t [d_\uparrow^\dagger Y^{mm} - f f^\dagger d_\uparrow^\dagger Y^{mm} - f d_\uparrow^\dagger f^\dagger Y^{mm}] \\
&= t [d_\uparrow^\dagger Y^{mm} + f d_\uparrow^\dagger f^\dagger Y^{mm} - f d_\uparrow^\dagger f^\dagger Y^{mm}] \\
[f^\dagger Y^{mm}, \Delta t f d_\uparrow^\dagger] &= t d_\uparrow^\dagger Y^{mm};
\end{aligned} \tag{A.36}$$

$$\begin{aligned}
[f^\dagger Y^{mm}, \Delta d_\uparrow f] &= \Delta [f^\dagger Y^{mm} d_\uparrow f - d_\uparrow f f^\dagger Y^{mm}] \\
&= \Delta [f^\dagger d_\uparrow f Y^{mm} - d_\uparrow f f^\dagger Y^{mm}] \\
&= \Delta [-d_\uparrow f^\dagger f Y^{mm} - d_\uparrow f f^\dagger Y^{mm}] \\
&= \Delta [-d_\uparrow (1 - f f^\dagger) Y^{mm} - d_\uparrow f f^\dagger Y^{mm}] \\
&= \Delta [-d_\uparrow Y^{mm} + d_\uparrow f f^\dagger Y^{mm} - d_\uparrow f f^\dagger Y^{mm}] \\
[f^\dagger Y^{mm}, \Delta d_\uparrow f] &= -\Delta d_\uparrow Y^{mm}.
\end{aligned} \tag{A.37}$$

Substituindo os resultados obtidos na Eq. (A.24), temos

$$\begin{aligned}
\omega^+ \langle \langle f^\dagger Y^{mm}; d_\sigma^\dagger \rangle \rangle &= \langle [f^\dagger Y^{mm}; d_\sigma^\dagger]_+ \rangle + \langle \langle [f^\dagger Y^{mm}, \mathcal{H}]; d_\sigma^\dagger \rangle \rangle \\
\omega^+ \langle \langle f^\dagger Y^{mm}; d_\sigma^\dagger \rangle \rangle &= -\varepsilon_M \langle \langle f^\dagger Y^{mm}; d_\sigma^\dagger \rangle \rangle + t \langle \langle d_\uparrow^\dagger Y^{mm}; d_\sigma^\dagger \rangle \rangle - \Delta \langle \langle d_\uparrow Y^{mm}; d_\sigma^\dagger \rangle \rangle \\
\omega^+ \langle \langle f^\dagger Y^{mm}; d_\sigma^\dagger \rangle \rangle + \varepsilon_M \langle \langle f^\dagger Y^{mm}; d_\sigma^\dagger \rangle \rangle &= t \langle \langle d_\uparrow^\dagger Y^{mm}; d_\sigma^\dagger \rangle \rangle - \Delta \langle \langle d_\uparrow Y^{mm}; d_\sigma^\dagger \rangle \rangle.
\end{aligned} \tag{A.38}$$

Calculando agora, $\langle \langle f Y^{mm}; d_\sigma^\dagger \rangle \rangle$

$$\omega^+ \langle \langle f Y^{mm}; d_\sigma^\dagger \rangle \rangle = \langle [f Y^{mm}; d_\sigma^\dagger]_+ \rangle + \langle \langle [f Y^{mm}, \mathcal{H}]; d_\sigma^\dagger \rangle \rangle. \tag{A.39}$$

Para o primeiro termo, temos

$$\begin{aligned}
[f Y^{mm}; d_\sigma^\dagger]_+ &= Y^{mm} [f d_\sigma^\dagger + d_\sigma^\dagger f] \\
&= Y^{mm} [-d_\sigma^\dagger f + d_\sigma^\dagger f] \\
[f^\dagger Y^{mm}; d_\sigma^\dagger]_+ &= 0.
\end{aligned} \tag{A.40}$$

Para o segundo termo, vamos primeiro calcular $[fY^{mm}, \mathcal{H}]$

$$\begin{aligned}
[fY^{mm}, \mathcal{H}] &= \left[fY^{mm}, \sum_{k\alpha\sigma'} \varepsilon_{k\alpha} c_{k\alpha\sigma'}^\dagger c_{k\alpha\sigma'} \right] + [fY^{mm}, \varepsilon_1 (n_\uparrow + n_\downarrow)] + \\
&+ \left[fY^{mm}, \sum_{k\alpha\sigma'} \left(V_{k\alpha} c_{k\alpha\sigma'}^\dagger d_{\sigma'} + V_{k\alpha}^* d_{\sigma'}^\dagger c_{k\alpha\sigma'} \right) \right] + \left[fY^{mm}, \frac{J}{2} \sum_m m n_\uparrow Y^{mm} \right] \\
&+ \left[fY^{mm}, \left(-\frac{J}{2} \sum_m m n_\downarrow Y^{mm} \right) \right] + [fY^{mm}, \varepsilon_M f^\dagger f] + [fY^{mm}, t d_\uparrow f^\dagger] \\
&+ [fY^{mm}, \Delta f^\dagger d_\uparrow^\dagger] + [fY^{mm}, t f d_\uparrow^\dagger] + [fY^{mm}, \Delta d_\uparrow f]. \tag{A.41}
\end{aligned}$$

Resolvendo a Eq. (A.41) termo a termo,

$$\left[fY^{mm}, \sum_{k\alpha\sigma'} \varepsilon_{k\alpha} c_{k\alpha\sigma'}^\dagger c_{k\alpha\sigma'} \right] = 0; \tag{A.42}$$

$$[fY^{mm}, \varepsilon_1 (n_\uparrow + n_\downarrow)] = 0; \tag{A.43}$$

$$\left[fY^{mm}, \sum_{k\alpha\sigma'} \left(V_{k\alpha} c_{k\alpha\sigma'}^\dagger d_{\sigma'} + V_{k\alpha}^* d_{\sigma'}^\dagger c_{k\alpha\sigma'} \right) \right] = 0; \tag{A.44}$$

$$\left[fY^{mm}, \frac{J}{2} \sum_m m n_\uparrow Y^{mm} \right] = 0; \tag{A.45}$$

$$\left[fY^{mm}, \left(-\frac{J}{2} \sum_m m n_\downarrow Y^{mm} \right) \right] = 0; \tag{A.46}$$

$$[fY^{mm}, t f d_\uparrow^\dagger] = 0; \tag{A.47}$$

$$[fY^{mm}, \Delta d_\uparrow f] = 0; \tag{A.48}$$

$$\begin{aligned}
[fY^{mm}, \varepsilon_M f^\dagger f] &= \varepsilon_M [fY^{mm} f^\dagger f' - f^\dagger f' fY^{mm}] \\
&= \varepsilon_M [f f^\dagger f' Y^{mm} - f^\dagger f' fY^{mm}] \\
&= \varepsilon_M [(1 - f^\dagger f) f' Y^{mm} - f^\dagger f' fY^{mm}] \\
&= \varepsilon_M [f' Y^{mm} - f^\dagger f f' Y^{mm} - f^\dagger f' fY^{mm}] \\
&= \varepsilon_M [f' Y^{mm} + f^\dagger f' fY^{mm} - f^\dagger f' fY^{mm}] \\
[fY^{mm}, \varepsilon_M f^\dagger f] &= \varepsilon_M f' Y^{mm} \\
[fY^{mm}, \varepsilon_M f^\dagger f] &= \varepsilon_M fY^{mm};
\end{aligned} \tag{A.49}$$

$$\begin{aligned}
[fY^{mm}, td_\uparrow f^\dagger] &= t [fY^{mm} d_\uparrow f^\dagger - d_\uparrow f^\dagger fY^{mm}] \\
&= t [f d_\uparrow f^\dagger Y^{mm} - d_\uparrow f^\dagger fY^{mm}] \\
&= t [-d_\uparrow f f^\dagger Y^{mm} - d_\uparrow f^\dagger fY^{mm}] \\
&= t [-d_\uparrow (1 - f^\dagger f) Y^{mm} - d_\uparrow f^\dagger fY^{mm}] \\
&= t [-d_\uparrow Y^{mm} + d_\uparrow f^\dagger fY^{mm} - d_\uparrow f^\dagger fY^{mm}] \\
[fY^{mm}, td_\uparrow f^\dagger] &= -td_\uparrow Y^{mm};
\end{aligned} \tag{A.50}$$

$$\begin{aligned}
[fY^{mm}, \Delta f^\dagger d_\uparrow^\dagger] &= \Delta [fY^{mm} f^\dagger d_\uparrow^\dagger - f^\dagger d_\uparrow^\dagger fY^{mm}] \\
&= \Delta [f f^\dagger d_\uparrow^\dagger Y^{mm} - f^\dagger d_\uparrow^\dagger fY^{mm}] \\
&= \Delta [(1 - f^\dagger f) d_\uparrow^\dagger Y^{mm} - f^\dagger d_\uparrow^\dagger fY^{mm}] \\
&= \Delta [d_\uparrow^\dagger Y^{mm} - f^\dagger f d_\uparrow^\dagger Y^{mm} - f^\dagger d_\uparrow^\dagger fY^{mm}] \\
&= \Delta [d_\uparrow^\dagger Y^{mm} + f^\dagger d_\uparrow^\dagger fY^{mm} - f^\dagger d_\uparrow^\dagger fY^{mm}] \\
[fY^{mm}, \Delta f^\dagger d_\uparrow^\dagger] &= \Delta d_\uparrow^\dagger Y^{mm}.
\end{aligned} \tag{A.51}$$

Então, substituindo todos os resultados obtidos, a Eq. (A.39) fica

$$\begin{aligned}
\omega^+ \langle \langle fY^{mm}; d_\sigma^\dagger \rangle \rangle &= \varepsilon_M \langle \langle fY^{mm}; d_\sigma^\dagger \rangle \rangle - t \langle \langle d_\uparrow Y^{mm}; d_\sigma^\dagger \rangle \rangle + \Delta \langle \langle d_\uparrow^\dagger Y^{mm}; d_\sigma^\dagger \rangle \rangle \\
\omega^+ \langle \langle fY^{mm}; d_\sigma^\dagger \rangle \rangle - \varepsilon_M \langle \langle fY^{mm}; d_\sigma^\dagger \rangle \rangle &= -t \langle \langle d_\uparrow Y^{mm}; d_\sigma^\dagger \rangle \rangle + \Delta \langle \langle d_\uparrow^\dagger Y^{mm}; d_\sigma^\dagger \rangle \rangle \\
(\omega^+ - \varepsilon_M) \langle \langle fY^{mm}; d_\sigma^\dagger \rangle \rangle &= -t \langle \langle d_\uparrow Y^{mm}; d_\sigma^\dagger \rangle \rangle + \Delta \langle \langle d_\uparrow^\dagger Y^{mm}; d_\sigma^\dagger \rangle \rangle
\end{aligned} \tag{A.52}$$

Agora, devemos calcular $\langle\langle d_{\uparrow}^{\dagger}Y^{mm}; d_{\sigma}^{\dagger}\rangle\rangle$.

$$\omega^+ \langle\langle d_{\uparrow}^{\dagger}Y^{mm}; d_{\sigma}^{\dagger}\rangle\rangle = \langle\langle [d_{\uparrow}^{\dagger}Y^{mm}; d_{\sigma}^{\dagger}]_+ \rangle\rangle + \langle\langle [d_{\uparrow}^{\dagger}Y^{mm}, \mathcal{H}]; d_{\sigma}^{\dagger}\rangle\rangle \quad (\text{A.53})$$

Para o primeiro termo, temos

$$\begin{aligned} [d_{\uparrow}^{\dagger}Y^{mm}; d_{\sigma}^{\dagger}]_+ &= Y^{mm} [d_{\uparrow}^{\dagger}d_{\sigma}^{\dagger} + d_{\sigma}^{\dagger}d_{\uparrow}^{\dagger}] \\ &= Y^{mm} [-d_{\sigma}^{\dagger}d_{\uparrow}^{\dagger} + d_{\sigma}^{\dagger}d_{\uparrow}^{\dagger}] \\ [d_{\uparrow}^{\dagger}Y^{mm}; d_{\sigma}^{\dagger}]_+ &= 0. \end{aligned} \quad (\text{A.54})$$

Para o segundo termo, vamos primeiro calcular $[d_{\uparrow}^{\dagger}Y^{mm}, \mathcal{H}]$

$$\begin{aligned} [d_{\uparrow}^{\dagger}Y^{mm}, \mathcal{H}] &= \left[d_{\uparrow}^{\dagger}Y^{mm}, \sum_{k\alpha\sigma'} \varepsilon_{k\alpha} c_{k\alpha\sigma'}^{\dagger} c_{k\alpha\sigma'} \right] + [d_{\uparrow}^{\dagger}Y^{mm}, \varepsilon_1 (n_{\uparrow} + n_{\downarrow})] \\ &+ \left[d_{\uparrow}^{\dagger}Y^{mm}, \sum_{k\alpha\sigma'} \left(V_{k\alpha} c_{k\alpha\sigma'}^{\dagger} d_{\sigma'} + V_{k\alpha}^* d_{\sigma'}^{\dagger} c_{k\alpha\sigma'} \right) \right] \\ &+ \left[d_{\uparrow}^{\dagger}Y^{mm}, \frac{J}{2} \sum_m m n_{\uparrow} Y^{mm} \right] + \left[d_{\uparrow}^{\dagger}Y^{mm}, \left(-\frac{J}{2} \sum_m m n_{\downarrow} Y^{mm} \right) \right] \\ &+ [d_{\uparrow}^{\dagger}Y^{mm}, \varepsilon_M f^{\dagger} f] + [d_{\uparrow}^{\dagger}Y^{mm}, t d_{\uparrow} f^{\dagger}] \\ &+ [d_{\uparrow}^{\dagger}Y^{mm}, \Delta f^{\dagger} d_{\uparrow}^{\dagger}] + [d_{\uparrow}^{\dagger}Y^{mm}, t f d_{\uparrow}^{\dagger}] + [d_{\uparrow}^{\dagger}Y^{mm}, \Delta d_{\uparrow} f]. \end{aligned} \quad (\text{A.55})$$

Resolvendo termo a termo a Eq. (A.55),

$$\left[d_{\uparrow}^{\dagger}Y^{mm}, \sum_{k\alpha\sigma'} \varepsilon_{k\alpha} c_{k\alpha\sigma'}^{\dagger} c_{k\alpha\sigma'} \right] = 0; \quad (\text{A.56})$$

$$[d_{\uparrow}^{\dagger}Y^{mm}, \varepsilon_M f^{\dagger} f] = 0; \quad (\text{A.57})$$

$$[d_{\uparrow}^{\dagger}Y^{mm}, \Delta f^{\dagger} d_{\uparrow}^{\dagger}] = 0; \quad (\text{A.58})$$

$$[d_{\uparrow}^{\dagger}Y^{mm}, t f d_{\uparrow}^{\dagger}] = 0; \quad (\text{A.59})$$

$$\begin{aligned}
\left[d_{\uparrow}^{\dagger} Y^{mm}, \varepsilon_1 (n_{\uparrow} + n_{\downarrow}) \right] &= \left[d_{\uparrow}^{\dagger} Y^{mm}, \varepsilon_1 (d_{\uparrow}^{\dagger'} d_{\uparrow} + d_{\downarrow}^{\dagger'} d_{\downarrow}) \right] \\
&= \varepsilon_1 \left[d_{\uparrow}^{\dagger} Y^{mm} (d_{\uparrow}^{\dagger'} d_{\uparrow} + d_{\downarrow}^{\dagger'} d_{\downarrow}) \right] \\
&= \varepsilon_1 \left[\left(d_{\uparrow}^{\dagger} Y^{mm} d_{\uparrow}^{\dagger'} d_{\uparrow} - d_{\uparrow}^{\dagger'} d_{\uparrow} d_{\uparrow}^{\dagger} Y^{mm} \right) \right] \\
&+ \varepsilon_1 \left[\left(d_{\uparrow}^{\dagger} Y^{mm} d_{\downarrow}^{\dagger'} d_{\downarrow} - d_{\downarrow}^{\dagger'} d_{\downarrow} d_{\uparrow}^{\dagger} Y^{mm} \right) \right] \\
&= \varepsilon_1 \left[\left(d_{\uparrow}^{\dagger} d_{\uparrow}^{\dagger'} d_{\uparrow} Y^{mm} - d_{\uparrow}^{\dagger'} d_{\uparrow} d_{\uparrow}^{\dagger} Y^{mm} \right) \right] \\
&+ \varepsilon_1 \left[\left(d_{\uparrow}^{\dagger} d_{\downarrow}^{\dagger'} d_{\downarrow} Y^{mm} - d_{\downarrow}^{\dagger'} d_{\downarrow} d_{\uparrow}^{\dagger} Y^{mm} \right) \right] \\
&= \varepsilon_1 \left[\left(-d_{\uparrow}^{\dagger'} d_{\uparrow}^{\dagger} d_{\uparrow} Y^{mm} - d_{\uparrow}^{\dagger'} d_{\uparrow} d_{\uparrow}^{\dagger} Y^{mm} \right) \right] \\
&- \varepsilon_1 \left[\left(d_{\downarrow}^{\dagger'} d_{\uparrow}^{\dagger} d_{\downarrow} Y^{mm} - d_{\downarrow}^{\dagger'} d_{\downarrow} d_{\uparrow}^{\dagger} Y^{mm} \right) \right] \\
&= \varepsilon_1 \left[\left(-d_{\uparrow}^{\dagger'} \left(1 - d_{\uparrow} d_{\uparrow}^{\dagger} \right) Y^{mm} - d_{\uparrow}^{\dagger'} d_{\uparrow} d_{\uparrow}^{\dagger} Y^{mm} \right) \right] \\
&+ \varepsilon_1 \left[\left(d_{\downarrow}^{\dagger'} d_{\downarrow} d_{\uparrow}^{\dagger} Y^{mm} - d_{\downarrow}^{\dagger'} d_{\downarrow} d_{\uparrow}^{\dagger} Y^{mm} \right) \right] \\
&= \varepsilon_1 \left[\left(-d_{\uparrow}^{\dagger'} \left(1 - d_{\uparrow} d_{\uparrow}^{\dagger} \right) Y^{mm} - d_{\uparrow}^{\dagger'} d_{\uparrow} d_{\uparrow}^{\dagger} Y^{mm} \right) \right] \\
&= \varepsilon_1 \left[\left(-d_{\uparrow}^{\dagger'} Y^{mm} + d_{\uparrow}^{\dagger'} d_{\uparrow} d_{\uparrow}^{\dagger} Y^{mm} - d_{\uparrow}^{\dagger'} d_{\uparrow} d_{\uparrow}^{\dagger} Y^{mm} \right) \right] \\
\left[d_{\uparrow}^{\dagger} Y^{mm}, \varepsilon_1 (n_{\uparrow} + n_{\downarrow}) \right] &= -\varepsilon_1 d_{\uparrow}^{\dagger'} Y^{mm}; \tag{A.60}
\end{aligned}$$

$$\begin{aligned}
\left[d_{\uparrow}^{\dagger} Y^{mm}, \sum_{k\alpha\sigma'} \left(V_{k\alpha} c_{k\alpha\sigma'}^{\dagger} d_{\sigma'} + V_{k\alpha}^* d_{\sigma'}^{\dagger} c_{k\alpha\sigma'} \right) \right] &= \sum_{k\alpha\sigma'} \left[d_{\uparrow}^{\dagger} Y^{mm}, \left(V_{k\alpha} c_{k\alpha\sigma'}^{\dagger} d_{\sigma'} + V_{k\alpha}^* d_{\sigma'}^{\dagger} c_{k\alpha\sigma'} \right) \right] \\
&= \sum_{k\alpha\sigma'} \left[\left[d_{\uparrow}^{\dagger} Y^{mm}, V_{k\alpha} c_{k\alpha\sigma'}^{\dagger} d_{\sigma'} \right] + \left[d_{\uparrow}^{\dagger} Y^{mm}, V_{k\alpha}^* d_{\sigma'}^{\dagger} c_{k\alpha\sigma'} \right] \right] \\
&= \sum_{k\alpha\sigma'} V_{k\alpha} \left[d_{\uparrow}^{\dagger} Y^{mm}, c_{k\alpha\sigma'}^{\dagger} d_{\sigma'} \right] + \sum_{k\alpha\sigma'} V_{k\alpha}^* \left[d_{\uparrow}^{\dagger} Y^{mm}, d_{\sigma'}^{\dagger} c_{k\alpha\sigma'} \right] \\
&= \sum_{k\alpha\sigma'} V_{k\alpha} \left[d_{\uparrow}^{\dagger} Y^{mm} c_{k\alpha\sigma'}^{\dagger} d_{\sigma'} - c_{k\alpha\sigma'}^{\dagger} d_{\sigma'} d_{\uparrow}^{\dagger} Y^{mm} \right] \\
&\quad + \sum_{k\alpha\sigma'} V_{k\alpha}^* \left[d_{\uparrow}^{\dagger} Y^{mm} d_{\sigma'}^{\dagger} c_{k\alpha\sigma'} - d_{\sigma'}^{\dagger} c_{k\alpha\sigma'} d_{\uparrow}^{\dagger} Y^{mm} \right] \\
&= \sum_{k\alpha\sigma'} V_{k\alpha} \left[d_{\uparrow}^{\dagger} c_{k\alpha\sigma'}^{\dagger} d_{\sigma'} Y^{mm} - c_{k\alpha\sigma'}^{\dagger} d_{\sigma'} d_{\uparrow}^{\dagger} Y^{mm} \right] \\
&\quad + \sum_{k\alpha\sigma'} V_{k\alpha}^* \left[d_{\uparrow}^{\dagger} d_{\sigma'}^{\dagger} c_{k\alpha\sigma'} Y^{mm} - d_{\sigma'}^{\dagger} c_{k\alpha\sigma'} d_{\uparrow}^{\dagger} Y^{mm} \right] \\
&= \sum_{k\alpha\sigma'} V_{k\alpha} \left[-c_{k\alpha\sigma'}^{\dagger} d_{\uparrow}^{\dagger} d_{\sigma'} Y^{mm} - c_{k\alpha\sigma'}^{\dagger} d_{\sigma'} d_{\uparrow}^{\dagger} Y^{mm} \right] \\
&\quad + \sum_{k\alpha\sigma'} V_{k\alpha}^* \left[-d_{\sigma'}^{\dagger} d_{\uparrow}^{\dagger} c_{k\alpha\sigma'} Y^{mm} - d_{\sigma'}^{\dagger} c_{k\alpha\sigma'} d_{\uparrow}^{\dagger} Y^{mm} \right] \\
&= \sum_{k\alpha\sigma'} V_{k\alpha} \left[-c_{k\alpha\sigma'}^{\dagger} d_{\uparrow}^{\dagger} d_{\sigma'} Y^{mm} - c_{k\alpha\sigma'}^{\dagger} d_{\sigma'} d_{\uparrow}^{\dagger} Y^{mm} \right] \\
&\quad + \sum_{k\alpha\sigma'} V_{k\alpha}^* \left[d_{\sigma'}^{\dagger} c_{k\alpha\sigma'} d_{\uparrow}^{\dagger} Y^{mm} - d_{\sigma'}^{\dagger} c_{k\alpha\sigma'} d_{\uparrow}^{\dagger} Y^{mm} \right] \\
&= \sum_{k\alpha\sigma'} V_{k\alpha} \left[-c_{k\alpha\sigma'}^{\dagger} \left(\delta_{\uparrow\sigma'} - d_{\sigma'} d_{\uparrow}^{\dagger} \right) Y^{mm} - c_{k\alpha\sigma'}^{\dagger} d_{\sigma'} d_{\uparrow}^{\dagger} Y^{mm} \right] \\
&= \sum_{k\alpha\sigma'} V_{k\alpha} \left[-c_{k\alpha\sigma'}^{\dagger} \delta_{\uparrow\sigma'} Y^{mm} + c_{k\alpha\sigma'}^{\dagger} d_{\sigma'} d_{\uparrow}^{\dagger} Y^{mm} \right] \\
&\quad - \sum_{k\alpha\sigma'} V_{k\alpha} \left[c_{k\alpha\sigma'}^{\dagger} d_{\sigma'} d_{\uparrow}^{\dagger} Y^{mm} \right] \\
\left[d_{\uparrow}^{\dagger} Y^{mm}, \sum_{k\alpha\sigma'} \left(V_{k\alpha} c_{k\alpha\sigma'}^{\dagger} d_{\sigma'} + V_{k\alpha}^* d_{\sigma'}^{\dagger} c_{k\alpha\sigma'} \right) \right] &= - \sum_{k\alpha\sigma'} V_{k\alpha} c_{k\alpha\sigma'}^{\dagger} Y^{mm}; \tag{A.61}
\end{aligned}$$

$$\begin{aligned}
\left[d_{\uparrow}^{\dagger} Y^{mm}, \frac{J}{2} \sum_{m'} m' n_{\uparrow} Y^{m'm'} \right] &= \frac{J}{2} \sum_{m'} m' \left[d_{\uparrow}^{\dagger} Y^{mm}, d_{\uparrow}^{\dagger'} d_{\uparrow} Y^{m'm'} \right] \\
&= \frac{J}{2} \sum_{m'} m' \left[d_{\uparrow}^{\dagger} Y^{mm} d_{\uparrow}^{\dagger'} d_{\uparrow} Y^{m'm'} - d_{\uparrow}^{\dagger'} d_{\uparrow} Y^{m'm'} d_{\uparrow}^{\dagger} Y^{mm} \right] \\
&= \frac{J}{2} \sum_{m'} m' \left[d_{\uparrow}^{\dagger} d_{\uparrow}^{\dagger'} d_{\uparrow} Y^{mm} Y^{m'm'} - d_{\uparrow}^{\dagger'} d_{\uparrow} d_{\uparrow}^{\dagger} Y^{m'm'} Y^{mm} \right] \\
&= \frac{J}{2} \sum_{m'} m' \left[d_{\uparrow}^{\dagger} d_{\uparrow}^{\dagger'} d_{\uparrow} \left(\delta_{mm'} Y^{mm'} \right) - d_{\uparrow}^{\dagger'} d_{\uparrow} d_{\uparrow}^{\dagger} \left(\delta_{m'm} Y^{m'm} \right) \right] \\
&= \frac{J}{2} \left[d_{\uparrow}^{\dagger} d_{\uparrow}^{\dagger'} d_{\uparrow} \left(\sum_{m'} m' \delta_{mm'} Y^{mm'} \right) - d_{\uparrow}^{\dagger'} d_{\uparrow} d_{\uparrow}^{\dagger} \left(\sum_{m'} m' \delta_{m'm} Y^{m'm} \right) \right] \\
&= \frac{J}{2} \left[d_{\uparrow}^{\dagger} d_{\uparrow}^{\dagger'} d_{\uparrow} (m Y^{mm}) - d_{\uparrow}^{\dagger'} d_{\uparrow} d_{\uparrow}^{\dagger} (m Y^{mm}) \right] \\
&= \frac{J}{2} \left[-d_{\uparrow}^{\dagger'} \left(1 - d_{\uparrow} d_{\uparrow}^{\dagger} \right) m Y^{mm} - d_{\uparrow}^{\dagger'} d_{\uparrow} d_{\uparrow}^{\dagger} m Y^{mm} \right] \\
&= \frac{J}{2} \left[-d_{\uparrow}^{\dagger'} m Y^{mm} + d_{\uparrow}^{\dagger'} d_{\uparrow} d_{\uparrow}^{\dagger} m Y^{mm} - d_{\uparrow}^{\dagger'} d_{\uparrow} d_{\uparrow}^{\dagger} m Y^{mm} \right] \\
\left[d_{\uparrow}^{\dagger} Y^{mm}, \frac{J}{2} \sum_{m'} m' n_{\uparrow} Y^{m'm'} \right] &= -\frac{J}{2} m d_{\uparrow}^{\dagger'} Y^{mm}; \tag{A.62}
\end{aligned}$$

$$\begin{aligned}
\left[d_{\uparrow}^{\dagger} Y^{mm}, -\frac{J}{2} \sum_{m'} m' n_{\downarrow} Y^{m'm'} \right] &= -\frac{J}{2} \sum_{m'} m' \left[d_{\uparrow}^{\dagger} Y^{mm}, d_{\downarrow}^{\dagger'} d_{\downarrow} Y^{m'm'} \right] \\
&= -\frac{J}{2} \sum_{m'} m' \left[d_{\uparrow}^{\dagger} Y^{mm} d_{\downarrow}^{\dagger'} d_{\downarrow} Y^{m'm'} - d_{\downarrow}^{\dagger'} d_{\downarrow} Y^{m'm'} d_{\uparrow}^{\dagger} Y^{mm} \right] \\
&= -\frac{J}{2} \sum_{m'} m' \left[d_{\uparrow}^{\dagger} d_{\downarrow}^{\dagger'} d_{\downarrow} Y^{mm} Y^{m'm'} - d_{\downarrow}^{\dagger'} d_{\downarrow} d_{\uparrow}^{\dagger} Y^{m'm'} Y^{mm} \right] \\
&= -\frac{J}{2} \sum_{m'} m' \left[d_{\uparrow}^{\dagger} d_{\downarrow}^{\dagger'} d_{\downarrow} \left(\delta_{mm'} Y^{mm'} \right) - d_{\downarrow}^{\dagger'} d_{\downarrow} d_{\uparrow}^{\dagger} \left(\delta_{m'm} Y^{m'm} \right) \right] \\
&= -\frac{J}{2} \left[d_{\uparrow}^{\dagger} d_{\downarrow}^{\dagger'} d_{\downarrow} \left(\sum_{m'} m' \delta_{mm'} Y^{mm'} \right) - d_{\downarrow}^{\dagger'} d_{\downarrow} d_{\uparrow}^{\dagger} \left(\sum_{m'} m' \delta_{m'm} Y^{m'm} \right) \right] \\
&= -\frac{J}{2} \left[d_{\uparrow}^{\dagger} d_{\downarrow}^{\dagger'} d_{\downarrow} \left(m' \delta_{mm'} Y^{mm'} \right) - d_{\downarrow}^{\dagger'} d_{\downarrow} d_{\uparrow}^{\dagger} \left(m' \delta_{m'm} Y^{m'm} \right) \right] \\
&= -\frac{J}{2} \left[-d_{\downarrow}^{\dagger'} d_{\uparrow}^{\dagger} d_{\downarrow} \left(m' \delta_{mm'} Y^{mm'} \right) - d_{\downarrow}^{\dagger'} d_{\downarrow} d_{\uparrow}^{\dagger} \left(m' \delta_{m'm} Y^{m'm} \right) \right] \\
&= -\frac{J}{2} \left[d_{\downarrow}^{\dagger'} d_{\downarrow} d_{\uparrow}^{\dagger} \left(m' \delta_{mm'} Y^{mm'} \right) - d_{\downarrow}^{\dagger'} d_{\downarrow} d_{\uparrow}^{\dagger} \left(m' \delta_{m'm} Y^{m'm} \right) \right] \\
\left[d_{\uparrow}^{\dagger} Y^{mm}, -\frac{J}{2} \sum_{m'} m' n_{\downarrow} Y^{m'm'} \right] &= 0; \tag{A.63}
\end{aligned}$$

$$\begin{aligned}
\left[d_{\uparrow}^{\dagger} Y^{mm}, t d_{\uparrow} f^{\dagger} \right] &= t \left[d_{\uparrow}^{\dagger} Y^{mm} d_{\uparrow} f^{\dagger} - d_{\uparrow} f^{\dagger} d_{\uparrow}^{\dagger} Y^{mm} \right] \\
&= t \left[d_{\uparrow}^{\dagger} d_{\uparrow} f^{\dagger} Y^{mm} - d_{\uparrow} f^{\dagger} d_{\uparrow}^{\dagger} Y^{mm} \right] \\
&= t \left[\left(1 - d_{\uparrow} d_{\uparrow}^{\dagger} \right) f^{\dagger} Y^{mm} - d_{\uparrow} f^{\dagger} d_{\uparrow}^{\dagger} Y^{mm} \right] \\
&= t \left[f^{\dagger} Y^{mm} - d_{\uparrow} d_{\uparrow}^{\dagger} f^{\dagger} Y^{mm} - d_{\uparrow} f^{\dagger} d_{\uparrow}^{\dagger} Y^{mm} \right] \\
&= t \left[f^{\dagger} Y^{mm} + d_{\uparrow} f^{\dagger} d_{\uparrow}^{\dagger} Y^{mm} - d_{\uparrow} f^{\dagger} d_{\uparrow}^{\dagger} Y^{mm} \right] \\
\left[d_{\uparrow}^{\dagger} Y^{mm}, t d_{\uparrow} f^{\dagger} \right] &= t f^{\dagger} Y^{mm};
\end{aligned} \tag{A.64}$$

$$\begin{aligned}
\left[d_{\uparrow}^{\dagger} Y^{mm}, \Delta d_{\uparrow} f \right] &= \Delta \left[d_{\uparrow}^{\dagger} Y^{mm} d_{\uparrow} f - d_{\uparrow} f d_{\uparrow}^{\dagger} Y^{mm} \right] \\
&= \Delta \left[d_{\uparrow}^{\dagger} d_{\uparrow} f Y^{mm} - d_{\uparrow} f d_{\uparrow}^{\dagger} Y^{mm} \right] \\
&= \Delta \left[\left(1 - d_{\uparrow} d_{\uparrow}^{\dagger} \right) f Y^{mm} - d_{\uparrow} f d_{\uparrow}^{\dagger} Y^{mm} \right] \\
&= \Delta \left[f Y^{mm} - d_{\uparrow} d_{\uparrow}^{\dagger} f Y^{mm} - d_{\uparrow} f d_{\uparrow}^{\dagger} Y^{mm} \right] \\
&= \Delta \left[f Y^{mm} + d_{\uparrow} f d_{\uparrow}^{\dagger} Y^{mm} - d_{\uparrow} f d_{\uparrow}^{\dagger} Y^{mm} \right] \\
\left[d_{\uparrow}^{\dagger} Y^{mm}, \Delta d_{\uparrow} f \right] &= \Delta f Y^{mm}.
\end{aligned} \tag{A.65}$$

Substituindo os resultados na Eq. (A.53), temos que

$$\begin{aligned}
\omega^+ \left\langle \left\langle d_{\uparrow}^{\dagger} Y^{mm}; d_{\sigma}^{\dagger} \right\rangle \right\rangle &= - \sum_{k\alpha\sigma'} V_{k\alpha} \left\langle \left\langle c_{k\alpha\sigma'}^{\dagger} Y^{mm}; d_{\sigma}^{\dagger} \right\rangle \right\rangle - \varepsilon_1 \left\langle \left\langle d_{\uparrow}^{\dagger} Y^{mm}; d_{\sigma}^{\dagger} \right\rangle \right\rangle \\
&- \frac{Jm}{2} \left\langle \left\langle d_{\uparrow}^{\dagger} Y^{mm}; d_{\sigma}^{\dagger} \right\rangle \right\rangle + t \left\langle \left\langle f^{\dagger} Y^{mm}; d_{\sigma}^{\dagger} \right\rangle \right\rangle + \Delta \left\langle \left\langle f Y^{mm}; d_{\sigma}^{\dagger} \right\rangle \right\rangle
\end{aligned}$$

$$\begin{aligned}
\left(\omega^+ + \varepsilon_1 + \frac{Jm}{2} \right) \left\langle \left\langle d_{\uparrow}^{\dagger} Y^{mm}; d_{\sigma}^{\dagger} \right\rangle \right\rangle &= - \sum_{k\alpha\sigma'} V_{k\alpha} \left\langle \left\langle c_{k\alpha\sigma'}^{\dagger} Y^{mm}; d_{\sigma}^{\dagger} \right\rangle \right\rangle \\
&+ t \left\langle \left\langle f^{\dagger} Y^{mm}; d_{\sigma}^{\dagger} \right\rangle \right\rangle + \Delta \left\langle \left\langle f Y^{mm}; d_{\sigma}^{\dagger} \right\rangle \right\rangle
\end{aligned} \tag{A.66}$$

Agora vamos calcular $\left\langle \left\langle c_{k\alpha\sigma}^{\dagger} Y^{mm}; d_{\sigma}^{\dagger} \right\rangle \right\rangle e \left\langle \left\langle c_{k\alpha\sigma} Y^{mm}; d_{\sigma}^{\dagger} \right\rangle \right\rangle$.

$$\omega^+ \left\langle \left\langle c_{k\alpha\sigma}^{\dagger} Y^{mm}; d_{\sigma}^{\dagger} \right\rangle \right\rangle = \left\langle \left[c_{k\alpha\sigma}^{\dagger} Y^{mm}; d_{\sigma}^{\dagger} \right]_+ \right\rangle + \left\langle \left\langle \left[c_{k\alpha\sigma}^{\dagger} Y^{mm}, \mathcal{H} \right]; d_{\sigma}^{\dagger} \right\rangle \right\rangle. \tag{A.67}$$

$$\begin{aligned}
\left[c_{k\alpha\sigma}^\dagger Y^{mm}, \mathcal{H} \right] &= \left[c_{k\alpha\sigma}^\dagger Y^{mm}, \sum_{k'\alpha'\sigma'} \varepsilon_{k'\alpha'} c_{k'\alpha'\sigma'}^\dagger c_{k'\alpha'\sigma'} \right] + \left[c_{k\alpha\sigma}^\dagger Y^{mm}, \varepsilon_1 (n_\uparrow + n_\downarrow) \right] \\
&+ \left[c_{k\alpha\sigma}^\dagger Y^{mm}, \sum_{k'\alpha'\sigma'} \left(V_{k'\alpha'} c_{k'\alpha'\sigma'}^\dagger d_{\sigma'} + V_{k'\alpha'}^* d_{\sigma'}^\dagger c_{k'\alpha'\sigma'} \right) \right] \\
&+ \left[c_{k\alpha\sigma}^\dagger Y^{mm}, \frac{J}{2} \sum_m m n_\uparrow Y^{mm} \right] + \left[c_{k\alpha\sigma}^\dagger Y^{mm}, \left(-\frac{J}{2} \sum_m m n_\downarrow Y^{mm} \right) \right] \\
&+ \left[c_{k\alpha\sigma}^\dagger Y^{mm}, \varepsilon_M f^\dagger f \right] + \left[c_{k\alpha\sigma}^\dagger Y^{mm}, t d_\uparrow f^\dagger \right] \\
&+ \left[c_{k\alpha\sigma}^\dagger Y^{mm}, \Delta f^\dagger d_\uparrow^\dagger \right] + \left[c_{k\alpha\sigma}^\dagger Y^{mm}, t f d_\uparrow^\dagger \right] + \left[c_{k\alpha\sigma}^\dagger Y^{mm}, \Delta d_\uparrow f \right]; \quad (\text{A.68})
\end{aligned}$$

$$\begin{aligned}
\left[c_{k\alpha\sigma}^\dagger Y^{mm}, \mathcal{H} \right] &= \left[c_{k\alpha\sigma}^\dagger Y^{mm}, \sum_{k'\alpha'\sigma'} \varepsilon_{k'\alpha'} c_{k'\alpha'\sigma'}^\dagger c_{k'\alpha'\sigma'} \right] \\
&+ \left[c_{k\alpha\sigma}^\dagger Y^{mm}, \sum_{k'\alpha'\sigma'} \left(V_{k'\alpha'} c_{k'\alpha'\sigma'}^\dagger d_{\sigma'} + V_{k'\alpha'}^* d_{\sigma'}^\dagger c_{k'\alpha'\sigma'} \right) \right]; \quad (\text{A.69})
\end{aligned}$$

$$\begin{aligned}
\left[c_{k\alpha\sigma}^\dagger Y^{mm}, \sum_{k'\alpha'\sigma'} \varepsilon_{k'\alpha'} c_{k'\alpha'\sigma'}^\dagger c_{k'\alpha'\sigma'} \right] &= \sum_{k'\alpha'\sigma'} \varepsilon_{k'\alpha'} \left[c_{k\alpha\sigma}^\dagger Y^{mm} c_{k'\alpha'\sigma'}^{\dagger'} c_{k'\alpha'\sigma'} \right] \\
&- \sum_{k'\alpha'\sigma'} \varepsilon_{k'\alpha'} \left[c_{k'\alpha'\sigma'}^{\dagger'} c_{k'\alpha'\sigma'} c_{k\alpha\sigma}^\dagger Y^{mm} \right] \\
&= \sum_{k'\alpha'\sigma'} \varepsilon_{k'\alpha'} \left[c_{k\alpha\sigma}^\dagger c_{k'\alpha'\sigma'}^{\dagger'} c_{k'\alpha'\sigma'} Y^{mm} \right] \\
&- \sum_{k'\alpha'\sigma'} \varepsilon_{k'\alpha'} \left[c_{k\alpha\sigma'}^{\dagger'} c_{k'\alpha'\sigma'} c_{k\alpha\sigma}^\dagger Y^{mm} \right] \\
&= \sum_{k'\alpha'\sigma'} \varepsilon_{k'\alpha'} \left[-c_{k'\alpha'\sigma'}^{\dagger'} c_{k\alpha\sigma}^\dagger c_{k'\alpha'\sigma'} Y^{mm} \right] \\
&- \sum_{k'\alpha'\sigma'} \varepsilon_{k'\alpha'} \left[c_{k\alpha\sigma'}^{\dagger'} c_{k'\alpha'\sigma'} c_{k\alpha\sigma}^\dagger Y^{mm} \right] \\
&= \sum_{k'\alpha'\sigma'} \varepsilon_{k'\alpha'} \left[-c_{k'\alpha'\sigma'}^{\dagger'} \left(\delta_{kk'} \delta_{\alpha\alpha'} \delta_{\sigma\sigma'} - c_{k'\alpha'\sigma'} c_{k\alpha\sigma}^\dagger \right) Y^{mm} \right] \\
&- \sum_{k'\alpha'\sigma'} \varepsilon_{k'\alpha'} \left[c_{k\alpha\sigma'}^{\dagger'} c_{k'\alpha'\sigma'} c_{k\alpha\sigma}^\dagger Y^{mm} \right] \\
&= \sum_{k'\alpha'\sigma'} \varepsilon_{k'\alpha'} \left[-c_{k'\alpha'\sigma'}^{\dagger'} \delta_{kk'} \delta_{\alpha\alpha'} \delta_{\sigma\sigma'} Y^{mm} \right] \\
&+ \sum_{k'\alpha'\sigma'} \varepsilon_{k'\alpha'} \left[c_{k\alpha\sigma'}^{\dagger'} c_{k'\alpha'\sigma'} c_{k\alpha\sigma}^\dagger Y^{mm} \right] \\
&= - \sum_{k\alpha\sigma'} \varepsilon_{k\alpha} c_{k'\alpha'\sigma'}^{\dagger'} \delta_{kk'} \delta_{\alpha\alpha'} \delta_{\sigma\sigma'} Y^{mm} \\
\left[c_{k\alpha\sigma}^\dagger Y^{mm}, \sum_{k\alpha\sigma'} \varepsilon_{k\alpha} c_{k\alpha\sigma'}^\dagger c_{k\alpha\sigma'} \right] &= -\varepsilon_{k\alpha} c_{k\alpha\sigma}^\dagger Y^{mm}; \tag{A.70}
\end{aligned}$$

$$\begin{aligned}
\left[c_{k\alpha\sigma}^\dagger Y^{mm}, \sum_{k'\alpha'\sigma'} \left(V_{k'\alpha'} c_{k'\alpha'\sigma'}^{\dagger'} d_{\sigma'} + V_{k'\alpha'}^* d_{\sigma'}^\dagger c_{k'\alpha'\sigma'} \right) \right] &= \sum_{k'\alpha'\sigma'} \left[c_{k\alpha\sigma}^\dagger Y^{mm}, \left(V_{k'\alpha'} c_{k'\alpha'\sigma'}^{\dagger'} d_{\sigma'} + V_{k'\alpha'}^* d_{\sigma'}^\dagger c_{k'\alpha'\sigma'} \right) \right] \\
&= \sum_{k'\alpha'\sigma'} V_{k'\alpha'} \left[c_{k\alpha\sigma}^\dagger Y^{mm}, c_{k'\alpha'\sigma'}^{\dagger'} d_{\sigma'} \right] \\
&+ \sum_{k'\alpha'\sigma'} V_{k'\alpha'}^* \left[c_{k\alpha\sigma}^\dagger Y^{mm}, d_{\sigma'}^\dagger c_{k'\alpha'\sigma'} \right] \\
&= \sum_{k'\alpha'\sigma'} V_{k'\alpha'} \left[c_{k\alpha\sigma}^\dagger Y^{mm} c_{k'\alpha'\sigma'}^{\dagger'} d_{\sigma'} \right] \\
&- \sum_{k'\alpha'\sigma'} V_{k'\alpha'} \left[c_{k'\alpha'\sigma'}^{\dagger'} d_{\sigma'} c_{k\alpha\sigma}^\dagger Y^{mm} \right] \\
&+ \sum_{k'\alpha'\sigma'} V_{k'\alpha'}^* \left[c_{k\alpha\sigma}^\dagger Y^{mm} d_{\sigma'}^\dagger c_{k'\alpha'\sigma'} \right] \\
&- \sum_{k'\alpha'\sigma'} V_{k'\alpha'}^* \left[d_{\sigma'}^\dagger c_{k'\alpha'\sigma'} c_{k\alpha\sigma}^\dagger Y^{mm} \right] \\
&= \sum_{k'\alpha'\sigma'} V_{k'\alpha'} \left[c_{k\alpha\sigma}^\dagger c_{k'\alpha'\sigma'}^{\dagger'} d_{\sigma'} Y^{mm} \right] \\
&- \sum_{k'\alpha'\sigma'} V_{k'\alpha'} \left[c_{k'\alpha'\sigma'}^{\dagger'} d_{\sigma'} c_{k\alpha\sigma}^\dagger Y^{mm} \right] \\
&+ \sum_{k'\alpha'\sigma'} V_{k'\alpha'}^* \left[c_{k\alpha\sigma}^\dagger d_{\sigma'}^\dagger c_{k'\alpha'\sigma'} Y^{mm} \right] \\
&- \sum_{k'\alpha'\sigma'} V_{k'\alpha'}^* \left[d_{\sigma'}^\dagger c_{k'\alpha'\sigma'} c_{k\alpha\sigma}^\dagger Y^{mm} \right] \\
&= \sum_{k'\alpha'\sigma'} V_{k'\alpha'} \left[-c_{k'\alpha'\sigma'}^{\dagger'} c_{k\alpha\sigma}^\dagger d_{\sigma'} Y^{mm} \right] \\
&- \sum_{k'\alpha'\sigma'} V_{k'\alpha'} \left[c_{k'\alpha'\sigma'}^{\dagger'} d_{\sigma'} c_{k\alpha\sigma}^\dagger Y^{mm} \right] \\
&+ \sum_{k'\alpha'\sigma'} V_{k'\alpha'}^* \left[-d_{\sigma'}^\dagger c_{k\alpha\sigma}^\dagger c_{k'\alpha'\sigma'} Y^{mm} \right] \\
&- \sum_{k'\alpha'\sigma'} V_{k'\alpha'}^* \left[d_{\sigma'}^\dagger c_{k'\alpha'\sigma'} c_{k\alpha\sigma}^\dagger Y^{mm} \right] \\
&= \sum_{k'\alpha'\sigma'} V_{k'\alpha'} \left[c_{k'\alpha'\sigma'}^{\dagger'} d_{\sigma'} c_{k\alpha\sigma}^\dagger Y^{mm} \right] \\
&- \sum_{k'\alpha'\sigma'} V_{k'\alpha'} \left[c_{k'\alpha'\sigma'}^{\dagger'} d_{\sigma'} c_{k\alpha\sigma}^\dagger Y^{mm} \right] \\
&+ \sum_{k'\alpha'\sigma'} V_{k'\alpha'}^* \left[-d_{\sigma'}^\dagger (\delta_{kk'} \delta_{\alpha\alpha'} \delta_{\sigma\sigma'}) Y^{mm} \right] \\
&+ \sum_{k'\alpha'\sigma'} V_{k'\alpha'}^* \left[-d_{\sigma'}^\dagger \left(c_{k'\alpha'\sigma'} c_{k\alpha\sigma}^\dagger \right) Y^{mm} \right] \\
&- \sum_{k'\alpha'\sigma'} V_{k'\alpha'}^* d_{\sigma'}^\dagger c_{k'\alpha'\sigma'} c_{k\alpha\sigma}^\dagger Y^{mm};
\end{aligned}$$

$$\begin{aligned}
\left[c_{k\alpha\sigma}^\dagger Y^{mm}, \sum_{k'\alpha'\sigma'} \left(V_{k'\alpha'} c_{k'\alpha'\sigma'}^\dagger d_{\sigma'} + V_{k'\alpha'}^* d_{\sigma'}^\dagger c_{k'\alpha'\sigma'} \right) \right] &= \sum_{k'\alpha'\sigma'} V_{k\alpha}^* \left[-d_{\sigma'}^\dagger \delta_{kk'} \delta_{\alpha\alpha'} \delta_{\sigma\sigma'} Y^{mm} \right] \\
&+ \sum_{k'\alpha'\sigma'} V_{k\alpha}^* \left[d_{\sigma'}^\dagger c_{k'\alpha'\sigma'} c_{k\alpha\sigma}^\dagger Y^{mm} \right] \\
&- \sum_{k'\alpha'\sigma'} V_{k'\alpha'}^* d_{\sigma'}^\dagger c_{k'\alpha'\sigma'} c_{k\alpha\sigma}^\dagger Y^{mm} \\
&= - \sum_{k'\alpha'\sigma'} V_{k'\alpha'}^* d_{\sigma'}^\dagger \delta_{kk'} \delta_{\alpha\alpha'} \delta_{\sigma\sigma'} Y^{mm} \\
\left[c_{k\alpha\sigma}^\dagger Y^{mm}, \sum_{k\alpha\sigma'} \left(V_{k'\alpha'} c_{k'\alpha'\sigma'}^\dagger d_{\sigma'} + V_{k'\alpha'}^* d_{\sigma'}^\dagger c_{k'\alpha'\sigma'} \right) \right] &= -V_{k'\alpha'}^* d_{\sigma'}^\dagger Y^{mm}; \tag{A.71}
\end{aligned}$$

$$\begin{aligned}
\omega^+ \left\langle \left\langle c_{k\alpha\sigma}^\dagger Y^{mm}; d_\sigma^\dagger \right\rangle \right\rangle &= - \left\langle \left\langle \varepsilon_{k\alpha} c_{k\alpha\sigma}^\dagger Y^{mm}; d_\sigma^\dagger \right\rangle \right\rangle - \left\langle \left\langle V_{k\alpha}^* d_\sigma^\dagger Y^{mm}; d_\sigma^\dagger \right\rangle \right\rangle \\
\omega^+ \left\langle \left\langle c_{k\alpha\sigma}^\dagger Y^{mm}; d_\sigma^\dagger \right\rangle \right\rangle + \varepsilon_{k\alpha} \left\langle \left\langle c_{k\alpha\sigma}^\dagger Y^{mm}; d_\sigma^\dagger \right\rangle \right\rangle &= - \left\langle \left\langle V_{k\alpha}^* d_\sigma^\dagger Y^{mm}; d_\sigma^\dagger \right\rangle \right\rangle \\
(\omega^+ + \varepsilon_{k\alpha}) \left\langle \left\langle c_{k\alpha\sigma}^\dagger Y^{mm}; d_\sigma^\dagger \right\rangle \right\rangle &= -V_{k\alpha}^* \left\langle \left\langle d_\sigma^\dagger Y^{mm}; d_\sigma^\dagger \right\rangle \right\rangle; \tag{A.72}
\end{aligned}$$

$$\left\langle \left\langle c_{k\alpha\sigma}^\dagger Y^{mm}; d_\sigma^\dagger \right\rangle \right\rangle = - \frac{V_{k\alpha}^*}{(\omega^+ + \varepsilon_{k\alpha})} \left\langle \left\langle d_\sigma^\dagger Y^{mm}; d_\sigma^\dagger \right\rangle \right\rangle; \tag{A.73}$$

$$\omega^+ \left\langle \left\langle c_{k\alpha\sigma} Y^{mm}; d_\sigma^\dagger \right\rangle \right\rangle = \left\langle \left[c_{k\alpha\sigma} Y^{mm}, d_\sigma^\dagger \right]_+ \right\rangle + \left\langle \left[c_{k\alpha\sigma} Y^{mm}, \mathcal{H} \right]; d_\sigma^\dagger \right\rangle; \tag{A.74}$$

$$\begin{aligned}
[c_{k\alpha\sigma} Y^{mm}, \mathcal{H}] &= \left[c_{k\alpha\sigma} Y^{mm}, \sum_{k'\alpha'\sigma'} \varepsilon_{k'\alpha'} c_{k'\alpha'\sigma'}^\dagger c_{k'\alpha'\sigma'} \right] + [c_{k\alpha\sigma} Y^{mm}, \varepsilon_1 (n_\uparrow + n_\downarrow)] \\
&+ \left[c_{k\alpha\sigma} Y^{mm}, \sum_{k'\alpha'\sigma'} \left(V_{k'\alpha'} c_{k'\alpha'\sigma'}^\dagger d_{\sigma'} + V_{k'\alpha'}^* d_{\sigma'}^\dagger c_{k'\alpha'\sigma'} \right) \right] \\
&+ \left[c_{k\alpha\sigma} Y^{mm}, \frac{J}{2} \sum_m m n_\uparrow Y^{mm} \right] + \left[c_{k\alpha\sigma} Y^{mm}, \left(-\frac{J}{2} \sum_m m n_\downarrow Y^{mm} \right) \right] \\
&+ [c_{k\alpha\sigma} Y^{mm}, \varepsilon_M f^\dagger f] + [c_{k\alpha\sigma} Y^{mm}, t d_\uparrow f^\dagger] \\
&+ [c_{k\alpha\sigma} Y^{mm}, \Delta f^\dagger d_\uparrow^\dagger] + [c_{k\alpha\sigma} Y^{mm}, t f d_\uparrow^\dagger] + [c_{k\alpha\sigma} Y^{mm}, \Delta d_\uparrow f]; \tag{A.75}
\end{aligned}$$

$$\begin{aligned}
[c_{k\alpha\sigma}Y^{mm}, \mathcal{H}] &= \left[c_{k\alpha\sigma}Y^{mm}, \sum_{k'\alpha'\sigma'} \varepsilon_{k'\alpha'} c_{k'\alpha'\sigma'}^\dagger c_{k'\alpha'\sigma'} \right] \\
&+ \left[c_{k\alpha\sigma}Y^{mm}, \sum_{k'\alpha'\sigma'} \left(V_{k'\alpha'} c_{k'\alpha'\sigma'}^\dagger d_{\sigma'} + V_{k'\alpha'}^* d_{\sigma'}^\dagger c_{k'\alpha'\sigma'} \right) \right]; \quad (\text{A.76})
\end{aligned}$$

$$\begin{aligned}
\left[c_{k\alpha\sigma}Y^{mm}, \sum_{k'\alpha'\sigma'} \varepsilon_{k'\alpha'} c_{k'\alpha'\sigma'}^\dagger c_{k'\alpha'\sigma'} \right] &= \sum_{k'\alpha'\sigma'} \varepsilon_{k'\alpha'} \left[c_{k\alpha\sigma}Y^{mm} c_{k'\alpha'\sigma'}^\dagger c_{k'\alpha'\sigma'} - c_{k'\alpha'\sigma'}^\dagger c_{k'\alpha'\sigma'} c_{k\alpha\sigma}Y^{mm} \right] \\
&= \sum_{k'\alpha'\sigma'} \varepsilon_{k'\alpha'} \left[c_{k\alpha\sigma} c_{k'\alpha'\sigma'}^\dagger c_{k'\alpha'\sigma'} Y^{mm} - c_{k'\alpha'\sigma'}^\dagger c_{k'\alpha'\sigma'} c_{k\alpha\sigma} Y^{mm} \right] \\
&= \sum_{k'\alpha'\sigma'} \varepsilon_{k'\alpha'} \left[\delta_{kk'} \delta_{\alpha\alpha'} \delta_{\sigma\sigma'} c_{k'\alpha'\sigma'}^\dagger Y^{mm} + c_{k'\alpha'\sigma'}^\dagger c_{k'\alpha'\sigma'} c_{k\alpha\sigma} Y^{mm} \right] \\
&- \sum_{k'\alpha'\sigma'} \varepsilon_{k'\alpha'} c_{k'\alpha'\sigma'}^\dagger c_{k'\alpha'\sigma'} c_{k\alpha\sigma} Y^{mm} \\
&= \sum_{k'\alpha'\sigma'} \varepsilon_{k'\alpha'} c_{k'\alpha'\sigma'} \delta_{kk'} \delta_{\alpha\alpha'} \delta_{\sigma\sigma'} Y^{mm} \\
\left[c_{k\alpha\sigma}^\dagger Y^{mm}, \sum_{k'\alpha'\sigma'} \varepsilon_{k'\alpha'} c_{k'\alpha'\sigma'}^\dagger c_{k'\alpha'\sigma'} \right] &= \varepsilon_{k'\alpha'} c_{k'\alpha'\sigma'} Y^{mm}; \quad (\text{A.77})
\end{aligned}$$

$$\begin{aligned}
\left[c_{k\alpha\sigma} Y^{mm}, \sum_{k\alpha\sigma'} \left(V_{k\alpha} c_{k\alpha\sigma'}^\dagger d_{\sigma'} + V_{k\alpha}^* d_{\sigma'}^\dagger c_{k\alpha\sigma'} \right) \right] &= \sum_{k'\alpha'\sigma'} \left[c_{k\alpha\sigma} Y^{mm}, \left(V_{k'\alpha'} c_{k'\alpha'\sigma'}^\dagger d_{\sigma'} + V_{k'\alpha'}^* d_{\sigma'}^\dagger c_{k'\alpha'\sigma'} \right) \right] \\
&= \sum_{k'\alpha'\sigma'} V_{k'\alpha'} \left[c_{k\alpha\sigma} Y^{mm}, c_{k'\alpha'\sigma'}^\dagger d_{\sigma'} \right] + \\
&+ \sum_{k'\alpha'\sigma'} V_{k'\alpha'}^* \left[c_{k\alpha\sigma} Y^{mm}, d_{\sigma'}^\dagger c_{k'\alpha'\sigma'} \right] \\
&= \sum_{k'\alpha'\sigma'} V_{k'\alpha'} \left[c_{k\alpha\sigma} Y^{mm} c_{k'\alpha'\sigma'}^\dagger d_{\sigma'} - c_{k'\alpha'\sigma'}^\dagger d_{\sigma'} c_{k\alpha\sigma} Y^{mm} \right] + \\
&+ \sum_{k'\alpha'\sigma'} V_{k'\alpha'}^* \left[c_{k\alpha\sigma} Y^{mm} d_{\sigma'}^\dagger c_{k'\alpha'\sigma'} - d_{\sigma'}^\dagger c_{k'\alpha'\sigma'} c_{k\alpha\sigma} Y^{mm} \right] \\
&= \sum_{k\alpha\sigma'} V_{k\alpha} \left[c_{k\alpha\sigma} c_{k\alpha\sigma'}^\dagger d_{\sigma'} Y^{mm} - c_{k\alpha\sigma'}^\dagger d_{\sigma'} c_{k\alpha\sigma} Y^{mm} \right] \\
&+ \sum_{k\alpha\sigma'} V_{k\alpha}^* \left[c_{k\alpha\sigma} d_{\sigma'}^\dagger c_{k'\alpha'\sigma'} Y^{mm} - d_{\sigma'}^\dagger c_{k'\alpha'\sigma'} c_{k\alpha\sigma} Y^{mm} \right] \\
&= \sum_{k\alpha\sigma'} V_{k\alpha} \left[\delta_{kk'} \delta_{\alpha\alpha'} \delta_{\sigma\sigma'} c_{k\alpha\sigma'}^\dagger c_{k\alpha\sigma} d_{\sigma'} Y^{mm} \right] \\
&- \sum_{k\alpha\sigma'} V_{k\alpha} \left[c_{k\alpha\sigma'}^\dagger d_{\sigma'} c_{k\alpha\sigma} Y^{mm} \right] \\
&+ \sum_{k\alpha\sigma'} V_{k\alpha}^* \left[-d_{\sigma'}^\dagger c_{k\alpha\sigma} c_{k'\alpha'\sigma'} Y^{mm} - d_{\sigma'}^\dagger c_{k'\alpha'\sigma'} c_{k\alpha\sigma} Y^{mm} \right] \\
&= \sum_{k'\alpha'\sigma'} V_{k'\alpha'} d_{\sigma'} \delta_{kk'} \delta_{\alpha\alpha'} \delta_{\sigma\sigma'} c_{k'\alpha'\sigma'}^\dagger Y^{mm} \\
\left[c_{k\alpha\sigma}^\dagger Y^{mm}, \sum_{k\alpha\sigma'} \left(V_{k\alpha} c_{k\alpha\sigma'}^\dagger d_{\sigma'} + V_{k\alpha}^* d_{\sigma'}^\dagger c_{k\alpha\sigma'} \right) \right] &= V_{k\alpha} d_{\sigma} Y^{mm}; \tag{A.78}
\end{aligned}$$

$$\begin{aligned}
\left[c_{k\alpha\sigma} Y^{mm}, \sum_{k\alpha\sigma'} \left(V_{k\alpha} c_{k\alpha\sigma'}^\dagger d_{\sigma'} + V_{k\alpha}^* d_{\sigma'}^\dagger c_{k\alpha\sigma'} \right) \right] &= \sum_{k'\alpha'\sigma'} \left[c_{k\alpha\sigma} Y^{mm}, \left(V_{k'\alpha'} c_{k'\alpha'\sigma'}^\dagger d_{\sigma'} + V_{k'\alpha'}^* d_{\sigma'}^\dagger c_{k'\alpha'\sigma'} \right) \right] \\
&= \sum_{k'\alpha'\sigma'} V_{k'\alpha'} \left[c_{k\alpha\sigma} Y^{mm}, c_{k'\alpha'\sigma'}^\dagger d_{\sigma'} \right] \\
&\quad + \sum_{k'\alpha'\sigma'} V_{k'\alpha'}^* \left[c_{k\alpha\sigma} Y^{mm}, d_{\sigma'}^\dagger c_{k'\alpha'\sigma'} \right] \\
&= \sum_{k'\alpha'\sigma'} V_{k'\alpha'} \left[c_{k\alpha\sigma} Y^{mm} c_{k'\alpha'\sigma'}^\dagger d_{\sigma'} - c_{k'\alpha'\sigma'}^\dagger d_{\sigma'} c_{k\alpha\sigma} Y^{mm} \right] \\
&\quad + \sum_{k'\alpha'\sigma'} V_{k'\alpha'}^* \left[c_{k\alpha\sigma} Y^{mm} d_{\sigma'}^\dagger c_{k'\alpha'\sigma'} - d_{\sigma'}^\dagger c_{k'\alpha'\sigma'} c_{k\alpha\sigma} Y^{mm} \right] \\
&= \sum_{k\alpha\sigma'} V_{k\alpha} \left[c_{k\alpha\sigma} c_{k\alpha\sigma'}^\dagger d_{\sigma'} Y^{mm} - c_{k\alpha\sigma'}^\dagger d_{\sigma'} c_{k\alpha\sigma} Y^{mm} \right] \\
&\quad + \sum_{k\alpha\sigma'} V_{k\alpha}^* \left[c_{k\alpha\sigma} d_{\sigma'}^\dagger c_{k'\alpha'\sigma'} Y^{mm} - d_{\sigma'}^\dagger c_{k'\alpha'\sigma'} c_{k\alpha\sigma} Y^{mm} \right] \\
&= \sum_{k\alpha\sigma'} V_{k\alpha} \left[\delta_{kk'} \delta_{\alpha\alpha'} \delta_{\sigma\sigma'} c_{k\alpha\sigma'}^\dagger c_{k\alpha\sigma} d_{\sigma'} Y^{mm} \right] \\
&\quad - \sum_{k\alpha\sigma'} V_{k\alpha} \left[c_{k\alpha\sigma'}^\dagger d_{\sigma'} c_{k\alpha\sigma} Y^{mm} \right] \\
&\quad + \sum_{k\alpha\sigma'} V_{k\alpha}^* \left[-d_{\sigma'}^\dagger c_{k\alpha\sigma} c_{k'\alpha'\sigma'} Y^{mm} - d_{\sigma'}^\dagger c_{k'\alpha'\sigma'} c_{k\alpha\sigma} Y^{mm} \right] \\
&= \sum_{k'\alpha'\sigma'} V_{k'\alpha'} d_{\sigma'} \delta_{kk'} \delta_{\alpha\alpha'} \delta_{\sigma\sigma'} c_{k'\alpha'\sigma'}^\dagger Y^{mm} \\
\left[c_{k\alpha\sigma}^\dagger Y^{mm}, \sum_{k\alpha\sigma'} \left(V_{k\alpha} c_{k\alpha\sigma'}^\dagger d_{\sigma'} + V_{k\alpha}^* d_{\sigma'}^\dagger c_{k\alpha\sigma'} \right) \right] &= V_{k\alpha} d_{\sigma} Y^{mm}; \tag{A.79}
\end{aligned}$$

$$\begin{aligned}
\omega^+ \langle \langle c_{k\alpha\sigma} Y^{mm}; d_{\sigma}^\dagger \rangle \rangle &= \langle \langle \varepsilon_{k\alpha} c_{k\alpha\sigma} Y^{mm}; d_{\sigma}^\dagger \rangle \rangle + \langle \langle V_{k\alpha}^* d_{\sigma} Y^{mm}; d_{\sigma}^\dagger \rangle \rangle \\
\omega^+ \langle \langle c_{k\alpha\sigma} Y^{mm}; d_{\sigma}^\dagger \rangle \rangle + \varepsilon_{k\alpha} \langle \langle c_{k\alpha\sigma} Y^{mm}; d_{\sigma}^\dagger \rangle \rangle &= \langle \langle V_{k\alpha} d_{\sigma} Y^{mm}; d_{\sigma}^\dagger \rangle \rangle \\
(\omega^+ + \varepsilon_{k\alpha}) \langle \langle c_{k\alpha\sigma} Y^{mm}; d_{\sigma}^\dagger \rangle \rangle &= V_{k\alpha} \langle \langle d_{\sigma} Y^{mm}; d_{\sigma}^\dagger \rangle \rangle; \tag{A.80}
\end{aligned}$$

$$\langle \langle c_{k\alpha\sigma} Y^{mm}; d_{\sigma}^\dagger \rangle \rangle = \frac{V_{k\alpha}}{(\omega^+ - \varepsilon_{k\alpha})} \langle \langle d_{\sigma} Y^{mm}; d_{\sigma}^\dagger \rangle \rangle. \tag{A.81}$$

Retomando a Eq. (A.23),

$$\begin{aligned}
\omega^+ \langle \langle d_\sigma Y^{mm}; d_\sigma^\dagger \rangle \rangle &= \langle Y^{mm} \rangle \\
&+ \sum_{k\alpha\sigma} V_{k\alpha}^* \left(\frac{V_{k\alpha}}{(\omega^+ - \varepsilon_{k\alpha})} \langle \langle d_\sigma Y^{mm}; d_\sigma^\dagger \rangle \rangle \right) \\
&+ \varepsilon_1 \delta_{\sigma\uparrow} \langle \langle d_\uparrow Y^{mm}; d_\sigma^\dagger \rangle \rangle + \varepsilon_1 \delta_{\sigma\downarrow} \langle \langle d_\downarrow Y^{mm}; d_\sigma^\dagger \rangle \rangle \\
&+ \frac{J}{2} \delta_{\sigma\uparrow} \langle \langle d_\uparrow m Y^{mm}; d_\sigma^\dagger \rangle \rangle \\
&- \frac{J}{2} \delta_{\sigma\downarrow} \langle \langle d_\downarrow m Y^{mm}; d_\sigma^\dagger \rangle \rangle \\
&- \Delta \delta_{\sigma\uparrow} \langle \langle f^\dagger Y^{mm}; d_\sigma^\dagger \rangle \rangle - t \delta_{\sigma\uparrow} \langle \langle f Y^{mm}; d_\sigma^\dagger \rangle \rangle \\
&= \langle Y^{mm} \rangle + \sum_{k\alpha\sigma} \frac{|V_{k\alpha}|^2}{(\omega^+ - \varepsilon_{k\alpha})} \langle \langle d_\sigma Y^{mm}; d_\sigma^\dagger \rangle \rangle \\
&+ \varepsilon_1 \delta_{\sigma\uparrow} \langle \langle d_\uparrow Y^{mm}; d_\sigma^\dagger \rangle \rangle + \varepsilon_1 \delta_{\sigma\downarrow} \langle \langle d_\downarrow Y^{mm}; d_\sigma^\dagger \rangle \rangle \\
&+ \frac{J}{2} \delta_{\sigma\uparrow} \langle \langle d_\uparrow m Y^{mm}; d_\sigma^\dagger \rangle \rangle \\
&- \frac{J}{2} \delta_{\sigma\downarrow} \langle \langle d_\downarrow m Y^{mm}; d_\sigma^\dagger \rangle \rangle \\
&- \Delta \delta_{\sigma\uparrow} \langle \langle f^\dagger Y^{mm}; d_\sigma^\dagger \rangle \rangle - t \delta_{\sigma\uparrow} \langle \langle f Y^{mm}; d_\sigma^\dagger \rangle \rangle \\
\omega^+ \langle \langle d_\sigma Y^{mm}; d_\sigma^\dagger \rangle \rangle - \sum_{k\alpha\sigma} \frac{|V_{k\alpha}|^2}{(\omega^+ - \varepsilon_{k\alpha})} \langle \langle d_\sigma Y^{mm}; d_\sigma^\dagger \rangle \rangle &= \langle Y^{mm} \rangle + \varepsilon_1 \delta_{\sigma\uparrow} \langle \langle d_\uparrow Y^{mm}; d_\sigma^\dagger \rangle \rangle \\
&+ \varepsilon_1 \delta_{\sigma\downarrow} \langle \langle d_\downarrow Y^{mm}; d_\sigma^\dagger \rangle \rangle \\
&+ \frac{J}{2} \delta_{\sigma\uparrow} \langle \langle d_\uparrow m Y^{mm}; d_\sigma^\dagger \rangle \rangle - \frac{J}{2} \delta_{\sigma\downarrow} \langle \langle d_\downarrow m Y^{mm}; d_\sigma^\dagger \rangle \rangle \\
&- \Delta \delta_{\sigma\uparrow} \langle \langle f^\dagger Y^{mm}; d_\sigma^\dagger \rangle \rangle - t \delta_{\sigma\uparrow} \langle \langle f Y^{mm}; d_\sigma^\dagger \rangle \rangle \\
\left[\omega^+ - \sum_{k\alpha\sigma} \frac{|V_{k\alpha}|^2}{(\omega^+ - \varepsilon_{k\alpha})} \right] \langle \langle d_\sigma Y^{mm}; d_\sigma^\dagger \rangle \rangle &= \langle Y^{mm} \rangle + \varepsilon_1 \delta_{\sigma\uparrow} \langle \langle d_\uparrow Y^{mm}; d_\sigma^\dagger \rangle \rangle \\
&+ \varepsilon_1 \delta_{\sigma\downarrow} \langle \langle d_\downarrow Y^{mm}; d_\sigma^\dagger \rangle \rangle \\
&+ \frac{J}{2} \delta_{\sigma\uparrow} \langle \langle d_\uparrow m Y^{mm}; d_\sigma^\dagger \rangle \rangle - \frac{J}{2} \delta_{\sigma\downarrow} \langle \langle d_\downarrow m Y^{mm}; d_\sigma^\dagger \rangle \rangle \\
&- \Delta \delta_{\sigma\uparrow} \langle \langle f^\dagger Y^{mm}; d_\sigma^\dagger \rangle \rangle \\
&- t \delta_{\sigma\uparrow} \langle \langle f Y^{mm}; d_\sigma^\dagger \rangle \rangle. \tag{A.82}
\end{aligned}$$

Agora, voltando para a Eq. (A.66), temos

$$\begin{aligned}
\left(\omega^+ + \varepsilon_1 + \frac{Jm}{2} \right) \langle \langle d_\uparrow^\dagger Y^{mm}; d_\sigma^\dagger \rangle \rangle &= - \sum_k V_k \left(- \frac{V_k^*}{(\omega^+ + \varepsilon_k)} \langle \langle d_\sigma^\dagger Y^{mm}; d_\sigma^\dagger \rangle \rangle \right) \\
&+ t \langle \langle f^\dagger Y^{mm}; d_\sigma^\dagger \rangle \rangle + \Delta \langle \langle f Y^{mm}; d_\sigma^\dagger \rangle \rangle. \tag{A.83}
\end{aligned}$$

$$\begin{aligned} \left(\omega^+ + \varepsilon_1 + \frac{Jm}{2} \right) \langle \langle d_{\uparrow}^{\dagger} Y^{mm}; d_{\sigma}^{\dagger} \rangle \rangle &= \sum_k \frac{|V_k|^2}{(\omega^+ + \varepsilon_k)} \langle \langle d_{\sigma}^{\dagger} Y^{mm}; d_{\sigma}^{\dagger} \rangle \rangle \\ &+ t \langle \langle f^{\dagger} Y^{mm}; d_{\sigma}^{\dagger} \rangle \rangle + \Delta \langle \langle f Y^{mm}; d_{\sigma}^{\dagger} \rangle \rangle. \end{aligned} \quad (\text{A.84})$$

A média estatística de $\langle Y^{mm} \rangle = 1/(2S+1)$, para cada $|m\rangle$ estados que compatilham a mesma probabilidade. Considerando $\sum_k |V_k|^2 / (\omega - \varepsilon_k + i\eta) = -i\Gamma$, então nós temos,

$$\begin{aligned} (\omega^+ + i\Gamma) \langle \langle d_{\sigma} Y^{mm}; d_{\sigma}^{\dagger} \rangle \rangle &= \frac{1}{(2S+1)} + \varepsilon_1 \delta_{\sigma\uparrow} \langle \langle d_{\uparrow} Y^{mm}; d_{\sigma}^{\dagger} \rangle \rangle + \varepsilon_1 \delta_{\sigma\downarrow} \langle \langle d_{\downarrow} Y^{mm}; d_{\sigma}^{\dagger} \rangle \rangle \\ &+ \frac{Jm}{2} \delta_{\sigma\uparrow} \langle \langle d_{\uparrow} Y^{mm}; d_{\sigma}^{\dagger} \rangle \rangle - \frac{Jm}{2} \delta_{\sigma\downarrow} \langle \langle d_{\downarrow} Y^{mm}; d_{\sigma}^{\dagger} \rangle \rangle \\ &- \Delta \delta_{\sigma\uparrow} \langle \langle f^{\dagger} Y^{mm}; d_{\sigma}^{\dagger} \rangle \rangle - t \delta_{\sigma\uparrow} \langle \langle f Y^{mm}; d_{\sigma}^{\dagger} \rangle \rangle, \end{aligned} \quad (\text{A.85})$$

$$\begin{aligned} \left(\omega^+ + \varepsilon_1 + \frac{Jm}{2} \right) \langle \langle d_{\uparrow}^{\dagger} Y^{mm}; d_{\sigma}^{\dagger} \rangle \rangle &= -i\Gamma \langle \langle d_{\sigma}^{\dagger} Y^{mm}; d_{\sigma}^{\dagger} \rangle \rangle \\ &+ t \langle \langle f^{\dagger} Y^{mm}; d_{\sigma}^{\dagger} \rangle \rangle + \Delta \langle \langle f Y^{mm}; d_{\sigma}^{\dagger} \rangle \rangle. \end{aligned} \quad (\text{A.86})$$

A.1.1 Funções de Green encontradas

$$\begin{aligned} (\omega^+ + i\Gamma) \langle \langle d_{\sigma} Y^{mm}; d_{\sigma}^{\dagger} \rangle \rangle &= \frac{1}{(2S+1)} + \varepsilon_1 \delta_{\sigma\uparrow} \langle \langle d_{\uparrow} Y^{mm}; d_{\sigma}^{\dagger} \rangle \rangle + \varepsilon_1 \delta_{\sigma\downarrow} \langle \langle d_{\downarrow} Y^{mm}; d_{\sigma}^{\dagger} \rangle \rangle \\ &+ \frac{Jm}{2} \delta_{\sigma\uparrow} \langle \langle d_{\uparrow} Y^{mm}; d_{\sigma}^{\dagger} \rangle \rangle - \frac{Jm}{2} \delta_{\sigma\downarrow} \langle \langle d_{\downarrow} Y^{mm}; d_{\sigma}^{\dagger} \rangle \rangle \\ &- \Delta \delta_{\sigma\uparrow} \langle \langle f^{\dagger} Y^{mm}; d_{\sigma}^{\dagger} \rangle \rangle - t \delta_{\sigma\uparrow} \langle \langle f Y^{mm}; d_{\sigma}^{\dagger} \rangle \rangle, \end{aligned} \quad (\text{A.87})$$

$$(\omega^+ + \varepsilon_M) \langle \langle f^{\dagger} Y^{mm}; d_{\sigma}^{\dagger} \rangle \rangle = t \langle \langle d_{\uparrow}^{\dagger} Y^{mm}; d_{\sigma}^{\dagger} \rangle \rangle - \Delta \langle \langle d_{\uparrow} Y^{mm}; d_{\sigma}^{\dagger} \rangle \rangle; \quad (\text{A.88})$$

$$(\omega^+ - \varepsilon_M) \langle \langle f Y^{mm}; d_{\sigma}^{\dagger} \rangle \rangle = -t \langle \langle d_{\uparrow} Y^{mm}; d_{\sigma}^{\dagger} \rangle \rangle + \Delta \langle \langle d_{\uparrow}^{\dagger} Y^{mm}; d_{\sigma}^{\dagger} \rangle \rangle; \quad (\text{A.89})$$

$$\begin{aligned} \left(\omega^+ + \varepsilon_1 + \frac{Jm}{2} \right) \langle \langle d_{\uparrow}^{\dagger} Y^{mm}; d_{\sigma}^{\dagger} \rangle \rangle &= -i\Gamma \langle \langle d_{\sigma}^{\dagger} Y^{mm}; d_{\sigma}^{\dagger} \rangle \rangle \\ &+ t \langle \langle f^{\dagger} Y^{mm}; d_{\sigma}^{\dagger} \rangle \rangle + \Delta \langle \langle f Y^{mm}; d_{\sigma}^{\dagger} \rangle \rangle. \end{aligned} \quad (\text{A.90})$$

A.1.2 Para o Spin-up

Vamos considerar $\sigma = \uparrow$

Para Eq. (A.87), temos

$$\begin{aligned} (\omega^+ + i\Gamma) \langle\langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle &= \frac{1}{(2S+1)} + \varepsilon_1 \langle\langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle + \frac{Jm}{2} \langle\langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle \\ &- \Delta \langle\langle f^{\dagger} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle - t \langle\langle f Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle. \end{aligned} \quad (\text{A.91})$$

Para a Eq. (A.88), temos

$$\begin{aligned} (\omega^+ + i\Gamma) \langle\langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle &= \frac{1}{(2S+1)} + \varepsilon_1 \langle\langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle + \frac{Jm}{2} \langle\langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle \\ &- \Delta \langle\langle f^{\dagger} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle - t \langle\langle f Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle. \end{aligned} \quad (\text{A.92})$$

Para a Eq. (A.89), temos

$$\langle\langle f^{\dagger} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle = \frac{t}{(\omega^+ + \varepsilon_M)} \langle\langle d_{\uparrow}^{\dagger} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle - \frac{\Delta}{(\omega^+ + \varepsilon_M)} \langle\langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle. \quad (\text{A.93})$$

Substituindo as Eqs. (A.88) e (A.89) na Eq. (A.87)

$$\begin{aligned}
(\omega^+ + i\Gamma) \langle\langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle &= \frac{1}{(2S+1)} + \varepsilon_1 \langle\langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle + \frac{Jm}{2} \langle\langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle \\
&- \Delta \langle\langle f^{\dagger} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle - t \langle\langle f Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle, \\
&= \frac{1}{(2S+1)} + \varepsilon_1 \langle\langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle + \frac{Jm}{2} \langle\langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle \\
&- \Delta \left[\frac{t}{(\omega^+ + \varepsilon_M)} \langle\langle d_{\uparrow}^{\dagger} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle - \frac{\Delta}{(\omega^+ + \varepsilon_M)} \langle\langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle \right] \\
&- t \left[-\frac{t}{(\omega^+ - \varepsilon_M)} \langle\langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle + \frac{\Delta}{(\omega^+ - \varepsilon_M)} \langle\langle d_{\uparrow}^{\dagger} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle \right] \\
\left(\omega^+ - \varepsilon_1 - \frac{Jm}{2} + i\Gamma \right) \langle\langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle &= \frac{1}{(2S+1)} \\
&- \Delta \left[\frac{t}{(\omega^+ + \varepsilon_M)} \langle\langle d_{\uparrow}^{\dagger} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle - \frac{\Delta}{(\omega^+ + \varepsilon_M)} \langle\langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle \right] \\
&- t \left[-\frac{t}{(\omega^+ - \varepsilon_M)} \langle\langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle + \frac{\Delta}{(\omega^+ - \varepsilon_M)} \langle\langle d_{\uparrow}^{\dagger} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle \right] \\
&= \frac{1}{(2S+1)} - \frac{\Delta t}{(\omega^+ + \varepsilon_M)} \langle\langle d_{\uparrow}^{\dagger} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle \\
&+ \frac{\Delta^2}{(\omega^+ + \varepsilon_M)} \langle\langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle \\
&+ \frac{t^2}{(\omega^+ - \varepsilon_M)} \langle\langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle - \frac{\Delta t}{(\omega^+ - \varepsilon_M)} \langle\langle d_{\uparrow}^{\dagger} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle \\
&= \frac{1}{(2S+1)} - \Delta t \left[\frac{1}{(\omega^+ + \varepsilon_M)} + \frac{1}{(\omega^+ - \varepsilon_M)} \right] \langle\langle d_{\uparrow}^{\dagger} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle \\
&+ \left[\frac{\Delta^2}{(\omega^+ + \varepsilon_M)} + \frac{t^2}{(\omega^+ - \varepsilon_M)} \right] \langle\langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle \\
&= \frac{1}{(2S+1)} - \Delta t \left[\frac{(\omega^+ - \varepsilon_M) + (\omega^+ + \varepsilon_M)}{(\omega^+ + \varepsilon_M)(\omega^+ - \varepsilon_M)} \right] \langle\langle d_{\uparrow}^{\dagger} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle \\
&+ \left[\frac{\Delta^2(\omega^+ - \varepsilon_M) + t^2(\omega^+ + \varepsilon_M)}{(\omega^+ + \varepsilon_M)(\omega^+ - \varepsilon_M)} \right] \langle\langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle \\
&= \frac{1}{(2S+1)} - \Delta t \left[\frac{2\omega^+}{(\omega^+)^2 - \varepsilon_M^2} \right] \langle\langle d_{\uparrow}^{\dagger} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle \\
&+ \left[\frac{\Delta^2\omega^+ - \Delta^2\varepsilon_M + t^2\omega^+ + t^2\varepsilon_M}{(\omega^+)^2 - \varepsilon_M^2} \right] \langle\langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle \\
&= \frac{1}{(2S+1)} - 2\Delta t \left[\frac{\omega^+}{(\omega^+)^2 - \varepsilon_M^2} \right] \langle\langle d_{\uparrow}^{\dagger} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle \quad (\text{A.94}) \\
&+ \left[\frac{\Delta^2\omega^+ - \Delta^2\varepsilon_M + t^2\omega^+ + t^2\varepsilon_M}{(\omega^+)^2 - \varepsilon_M^2} \right] \langle\langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle. \quad (\text{A.95})
\end{aligned}$$

Podemos escrever $\omega^+ = \omega + i\eta$. Então,

$$\begin{aligned} \left(\omega^+ - \varepsilon_1 - \frac{Jm}{2} + i\Gamma \right) \langle \langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \rangle \rangle &= \frac{1}{(2S+1)} 2t\Delta \left[\frac{(\omega + i\eta^+)}{\omega^2 - \varepsilon_M^2 + 2i\omega\eta^+ - (\eta^+)^2} \right] \langle \langle d_{\uparrow}^{\dagger} Y^{mm}; d_{\uparrow}^{\dagger} \rangle \rangle \\ &+ \left[\frac{\omega^+ (\Delta^2 + t^2) + \varepsilon_M (t^2 - \Delta^2)}{\omega^2 - \varepsilon_M^2 + 2i\omega\eta^+ - (\eta^+)^2} \right] \langle \langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \rangle \rangle. \end{aligned} \quad (\text{A.96})$$

Vamos considerar agora,

$$K_+ = \frac{(\omega + i\eta^+) (\Delta^2 + t^2) + \varepsilon_M (t^2 - \Delta^2)}{\omega^2 - \varepsilon_M^2 + 2i\omega\eta^+ - (\eta^+)^2}. \quad (\text{A.97})$$

Vamos considerar também,

$$K_{MFs} = \frac{(\omega + i\eta^+)}{\omega^2 - \varepsilon_M^2 + 2i\omega\eta^+ - (\eta^+)^2}, \quad (\text{A.98})$$

então, podemos reescrever a Eq. (A.87) como

$$\begin{aligned} \left(\omega^+ - \varepsilon_1 - \frac{Jm}{2} + i\Gamma \right) \langle \langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \rangle \rangle &= \frac{1}{(2S+1)} \\ &- 2t\Delta K_{MFs} \langle \langle d_{\uparrow}^{\dagger} Y^{mm}; d_{\uparrow}^{\dagger} \rangle \rangle \\ &+ K_+ \langle \langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \rangle \rangle \\ \left(\omega^+ - \varepsilon_1 - \frac{Jm}{2} + i\Gamma \right) \langle \langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \rangle \rangle - K_+ \langle \langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \rangle \rangle &= \frac{1}{(2S+1)} - 2t\Delta K_{MFs} \langle \langle d_{\uparrow}^{\dagger} Y^{mm}; d_{\uparrow}^{\dagger} \rangle \rangle \\ \left(\omega^+ - \varepsilon_1 - \frac{Jm}{2} + i\Gamma - K_+ \right) \langle \langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \rangle \rangle &= \frac{1}{(2S+1)} \\ &- 2t\Delta K_{MFs} \langle \langle d_{\uparrow}^{\dagger} Y^{mm}; d_{\uparrow}^{\dagger} \rangle \rangle. \end{aligned} \quad (\text{A.99})$$

Agora, substituindo o termo $\langle\langle d_{\uparrow}^{\dagger} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle$, temos

$$\begin{aligned}
\left(\omega^+ + \varepsilon_1 + \frac{Jm}{2}\right) \langle\langle d_{\uparrow}^{\dagger} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle &= -i\Gamma \langle\langle d_{\uparrow}^{\dagger} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle \\
&+ t \langle\langle f^{\dagger} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle + \Delta \langle\langle f Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle \\
\left(\omega^+ + \varepsilon_1 + \frac{Jm}{2} + i\Gamma\right) \langle\langle d_{\uparrow}^{\dagger} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle &= t \langle\langle f^{\dagger} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle + \Delta \langle\langle f Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle \\
\left(\omega^+ + \varepsilon_1 + \frac{Jm}{2} + i\Gamma\right) \langle\langle d_{\uparrow}^{\dagger} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle &= t \left(\frac{t}{(\omega^+ + \varepsilon_M)} \langle\langle d_{\uparrow}^{\dagger} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle - \frac{\Delta}{(\omega^+ + \varepsilon_M)} \langle\langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle \right) \\
&+ \Delta \left(\frac{\Delta}{(\omega^+ - \varepsilon_M)} \langle\langle d_{\uparrow}^{\dagger} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle - \frac{t}{(\omega^+ - \varepsilon_M)} \langle\langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle \right) \\
&= \frac{t^2}{(\omega^+ + \varepsilon_M)} \langle\langle d_{\uparrow}^{\dagger} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle - \frac{t\Delta}{(\omega^+ + \varepsilon_M)} \langle\langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle \\
&+ \frac{\Delta^2}{(\omega^+ - \varepsilon_M)} \langle\langle d_{\uparrow}^{\dagger} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle - \frac{\Delta t}{(\omega^+ - \varepsilon_M)} \langle\langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle \\
&= \left[\frac{t^2}{(\omega^+ + \varepsilon_M)} + \frac{\Delta^2}{(\omega^+ - \varepsilon_M)} \right] \langle\langle d_{\uparrow}^{\dagger} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle \\
&- \left[\frac{t\Delta}{(\omega^+ + \varepsilon_M)} + \frac{\Delta t}{(\omega^+ - \varepsilon_M)} \right] \langle\langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle \\
&= \left[\frac{t^2(\omega^+ - \varepsilon_M) + \Delta^2(\omega^+ + \varepsilon_M)}{(\omega^+ + \varepsilon_M)(\omega^+ - \varepsilon_M)} \right] \langle\langle d_{\uparrow}^{\dagger} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle \\
&- t\Delta \left[\frac{(\omega^+ - \varepsilon_M) + (\omega^+ + \varepsilon_M)}{(\omega^+ + \varepsilon_M)(\omega^+ - \varepsilon_M)} \right] \langle\langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle \\
&= \left[\frac{t^2\omega^+ - t^2\varepsilon_M + \Delta^2\omega^+ + \Delta^2\varepsilon_M}{(\omega^+)^2 - \varepsilon_M^2} \right] \langle\langle d_{\uparrow}^{\dagger} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle \\
&- t\Delta \left[\frac{(\omega^+ - \varepsilon_M) + (\omega^+ + \varepsilon_M)}{(\omega^+)^2 - \varepsilon_M^2} \right] \langle\langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle \\
&= \left[\frac{\omega^+(t^2 + \Delta^2) - \varepsilon_M(t^2 - \Delta^2)}{(\omega^+)^2 - \varepsilon_M^2} \right] \langle\langle d_{\uparrow}^{\dagger} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle \\
&- t\Delta \left[\frac{2\omega^+}{(\omega^+)^2 - \varepsilon_M^2} \right] \langle\langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle \\
&= \left[\frac{\omega^+(t^2 + \Delta^2) - \varepsilon_M(t^2 - \Delta^2)}{(\omega^+)^2 - \varepsilon_M^2} \right] \langle\langle d_{\uparrow}^{\dagger} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle \\
&- 2t\Delta \left[\frac{\omega^+}{(\omega^+)^2 - \varepsilon_M^2} \right] \langle\langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle \\
&= \left[\frac{(\omega + i\eta^+)(t^2 + \Delta^2) - \varepsilon_M(t^2 - \Delta^2)}{\omega^2 + 2\omega i\eta^+ - (\eta^+)^2 - \varepsilon_M^2} \right] \langle\langle d_{\uparrow}^{\dagger} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle \\
&- 2t\Delta \left[\frac{(\omega + i\eta^+)}{\omega^2 + 2\omega i\eta^+ - (\eta^+)^2 - \varepsilon_M^2} \right] \langle\langle d_{\uparrow} Y^{mm}; d_{\uparrow}^{\dagger} \rangle\rangle, \quad (\text{A.100})
\end{aligned}$$

sendo,

$$K_- = \frac{(\omega + i\eta^+)(t^2 + \Delta^2) - \varepsilon_M(t^2 - \Delta^2)}{\omega^2 - \varepsilon_M^2 + 2i\omega\eta^+ - (\eta^+)^2}. \quad (\text{A.101})$$

Então, a Eq. (A.99), fica

$$\begin{aligned} \left(\omega^+ + \varepsilon_1 + \frac{Jm}{2} + i\Gamma\right) \langle\langle d_\uparrow^\dagger Y^{mm}; d_\uparrow^\dagger \rangle\rangle &= K_- \langle\langle d_\uparrow^\dagger Y^{mm}; d_\uparrow^\dagger \rangle\rangle \\ &\quad - 2t\Delta K_{MFs} \langle\langle d_\uparrow Y^{mm}; d_\uparrow^\dagger \rangle\rangle \\ \left(\omega^+ + \varepsilon_1 + \frac{Jm}{2} + i\Gamma - K_- \right) \langle\langle d_\uparrow^\dagger Y^{mm}; d_\uparrow^\dagger \rangle\rangle &= -2t\Delta K_{MFs} \langle\langle d_\uparrow Y^{mm}; d_\uparrow^\dagger \rangle\rangle \end{aligned}$$

$$\langle\langle d_\uparrow^\dagger Y^{mm}; d_\uparrow^\dagger \rangle\rangle = -\frac{2t\Delta K_{MFs}}{(\omega^+ + \varepsilon_1 + \frac{Jm}{2} + i\Gamma - K_-)} \langle\langle d_\uparrow Y^{mm}; d_\uparrow^\dagger \rangle\rangle. \quad (\text{A.102})$$

Substituindo a Eq. (A.102) na Eq. (A.99), temos

$$\begin{aligned} \left(\omega^+ - \varepsilon_1 - \frac{Jm}{2} + i\Gamma - K_+\right) \langle\langle d_\uparrow Y^{mm}; d_\uparrow^\dagger \rangle\rangle &= \frac{1}{(2S+1)} - 2t\Delta K_{MFs} \langle\langle d_\uparrow^\dagger Y^{mm}; d_\uparrow^\dagger \rangle\rangle \\ &= \frac{1}{(2S+1)} \\ &\quad - 2t\Delta K_{MFs} \left[-\frac{2t\Delta K_{MFs}}{(\omega^+ + \varepsilon_1 + \frac{Jm}{2} + i\Gamma - K_-)} \langle\langle d_\uparrow Y^{mm}; d_\uparrow^\dagger \rangle\rangle \right] \\ &= \frac{1}{(2S+1)} \\ &\quad + \frac{(2t\Delta K_{MFs})^2}{(\omega^+ + \varepsilon_1 + \frac{Jm}{2} + i\Gamma - K_-)} \langle\langle d_\uparrow Y^{mm}; d_\uparrow^\dagger \rangle\rangle, \end{aligned} \quad (\text{A.103})$$

sendo,

$$\tilde{K}_m = \frac{K_{MFs}}{(\omega^+ + \varepsilon_1 + \frac{Jm}{2} + i\Gamma - K_-)}. \quad (\text{A.104})$$

Reescrever a Eq. (A.102),

$$\left(\omega^+ - \varepsilon_1 - \frac{Jm}{2} + i\Gamma - K_+\right) \langle\langle d_\uparrow Y^{mm}; d_\uparrow^\dagger \rangle\rangle = \frac{1}{(2S+1)} + (2t\Delta)^2 K_{MFs} \tilde{K}_m \langle\langle d_\uparrow Y^{mm}; d_\uparrow^\dagger \rangle\rangle$$

$$\left(\omega^+ - \varepsilon_1 - \frac{Jm}{2} + i\Gamma - K_+ - (2t\Delta)^2 K_{MFs} \tilde{K}_m\right) \langle\langle d_\uparrow Y^{mm}; d_\uparrow^\dagger \rangle\rangle = \frac{1}{(2S+1)}. \quad (\text{A.105})$$

Para simplificar a escrita, vamos considerar

$$\mathcal{Y}_{MFs}^m = K_+ + (2t\Delta)^2 K_{MFs} \tilde{K}_m, \quad (\text{A.106})$$

então

$$\langle\langle d_\uparrow Y^{mm}; d_\uparrow^\dagger \rangle\rangle = \frac{1}{(2S+1)} \frac{1}{\left(\omega^+ - \varepsilon_1 - \frac{Jm}{2} + i\Gamma - \mathcal{Y}_{MFs}^m\right)}. \quad (\text{A.107})$$

A Função de Green é dada por $G_\sigma^r(\omega) = \langle\langle d_\sigma; d_\sigma^\dagger \rangle\rangle = \sum_m \langle\langle d_\sigma Y^{mm}; d_\sigma^\dagger \rangle\rangle$, então a Eq. (A.107), fica

$$G_\uparrow^r = \sum_m \langle\langle d_\uparrow Y^{mm}; d_\uparrow^\dagger \rangle\rangle = \frac{1}{(2S+1)} \sum_m \frac{1}{\left(\omega^+ - \varepsilon_1 - \frac{Jm}{2} + i\Gamma - \mathcal{Y}_{MFs}^m\right)}.$$

$$\tilde{K}_m = \frac{K_{MFs}}{\left(\omega^+ + \varepsilon_1 + \frac{Jm}{2} + i\Gamma - K_-\right)} \quad (\text{A.108})$$

$$K_- = \frac{(\omega + i\eta^+)(t^2 + \Delta^2) - \varepsilon_M(t^2 - \Delta^2)}{\omega^2 + 2i\omega\eta^+ - (\eta^+)^2 - \varepsilon_M^2} \quad (\text{A.109})$$

$$K_{MFs} = \frac{(\omega + i\eta^+)}{\omega^2 + 2i\omega\eta^+ - (\eta^+)^2 - \varepsilon_M^2} \quad (\text{A.110})$$

A.2 Artigo publicado

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Fractionalization of Majorana-Ising-type quasiparticle excitations

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We theoretically investigate the spectral properties of a quantum impurity (QI) hosting the here proposed Majorana-Ising-type quasiparticle (MIQ) excitation. It arises from the coupling between a finite topological superconductor (TSC) based on a chain of magnetic adatoms-superconducting hybrid system and an integer large spin S flanking the QI. Noteworthy, the spin S couples to the QI via the Ising-type exchange interaction. As the Majorana zero-modes (MZMs) at the edges of the TSC chain are overlapped, we counterintuitively find a regime wherein the Ising term modulates the localization of a fractionalized and resonant MZM at the QI site. Interestingly enough, the fermionic nature of this state is revealed as purely of electron tunneling-type and most astonishingly, it has the Andreev conductance completely null in its birth. Therefore, we find that a resonant edge state appears as a zero-mode and discuss it in terms of a *poor man's Majorana*[Nature 614, 445 (2023)].

I. INTRODUCTION

Majorana fermions are peculiar particles equal to their own antiparticles described by real solutions of the Dirac equation[1]. In condensed matter Physics, such fermions rise as quasiparticle excitations usually quoted as Majorana zero-modes (MZMs), which are found attached to the boundaries of topological superconductors (TSCs)[2–31]. Astonishingly, since the theoretical Kitaev seminal proposal of p -wave superconductivity[32], MZMs are notably coveted due to their attribution as building-blocks for the highly pursued fault-tolerant topological quantum computing. Thereafter, in the last years, such excitations have received astounding focus from both communities working with quantum science and technology.

Interestingly enough, theoretical predictions point out that the fractional zero-bias peak (ZBP) in transport evaluations through quantum dots, which is given by the conductance $\mathcal{G}_{\text{Total}}(0) = \frac{e^2}{2h}$ [2–4], could have its origin from both the system topological nontrivial regime, where two MZMs emerge spatially far apart at the edges of a TSC[3, 4], as well as in the corresponding trivial, which could exhibit, for instance, Andreev bound states (ABSs)[33, 34]. In this regard, we highlight Ref.[35], which by treating the TSC within the theoretical framework of the Oreg-Lutchyn Hamiltonian[9], allows a detailed and systematic analysis on the formation of MZMs versus ABSs issue. In parallel, effective models[3, 33, 36], despite their simplifications, are used to capture, with a quite good accuracy, the corresponding low-energy Physics encoded by models such as that in Ref.[9] and the Kitaev Hamiltonian[32].

Back to the issue of the topological nontrivial regime, not less important, once an ordinary fermion can be

decomposed into two MZMs, is the amplitude $1/2$ in $\mathcal{G}_{\text{Total}}(0)$, the hallmark of the fractionalization of the quantum of conductance $\frac{e^2}{h}$, thus giving rise to the concept of fractionalized electronic zero-frequency spectral weight, which indeed reveals, the MZM “half-fermionic” nature[4]. This aforementioned fingerprint is expected to show up in engineered platforms that combine conventional s -wave superconductivity and spin-texture [see Refs.[37–39] and Fig.1(a)]. As aftermath, the p -wave superconductivity becomes feasible, thus allowing the experimental realization of the spinless Kitaev wire, which is indeed, a TSC in 1D[7, 25, 27, 32, 40–43]. For such an accomplishment, we highlight two practical recipes based on the Oreg-Lutchyn proposal[9], which have the following ingredients: (i) a semiconducting nanowire, with strong spin-orbit coupling (SOC) and under a magnetic field, should be deposited on top of an s -wave superconductor[25, 29–31, 40, 41, 44] or (ii) a linear chain of magnetic adatoms with exchange interactions should be hosted by an s -wave superconductor with strong SOC[13, 18, 37–39, 45–51]. In both the situations, the s -wave superconductors with singlet Cooper pairing lead to the so-called superconducting proximity effect, which is pivotal to carry forward the superconducting (SC) character into such manufactured Kitaev wires. Thus, the Zeeman field from the previous recipes (i) and (ii), together with the magnified SOC from such quantum materials, establish a synergy that stabilizes the system spin-texture. Consequently, the triplet Cooper pairing for the p -wave superconductivity, as well.

Particularly in the topological nontrivial regime of such setups, these Majorana quasiparticle excitations emerge ideally, i.e., as MZMs decoupled from each other and localized on the boundaries of the TSC. Due to this decoupling from their environment, MZMs are regarded robust against perturbations, once they are topologically protected by the SC gap. Thus, MZMs become promising candidates for a quantum computing free of the decoher-

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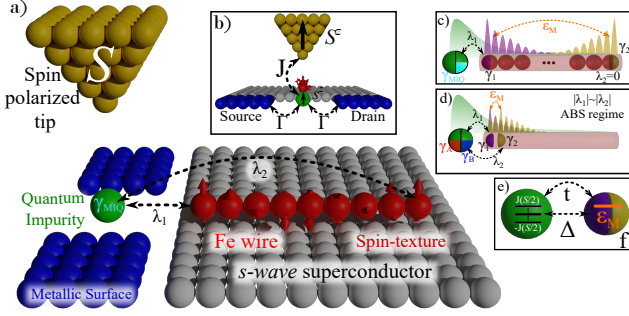


Figure 1. (a) Proposed device expected to show a Majorana-Ising-type quasiparticle (MIQ) excitation γ_{MIQ} localized at the quantum impurity (QI) site. The γ_{MIQ} leads to a zero-bias conductance peak $\mathcal{G}_{\text{MIQ}}(0) = \frac{e^2}{4h}$ due to the QI placed between source and drain leads, but the total conductance is still $\mathcal{G}_{\text{Total}}(0) = \frac{e^2}{2h}$. This occurs once a genuine electron tunneling process is present and there is a complete lack of local Andreev reflection. It can be performed by considering the QI simultaneously coupled to a spin-polarized tip with an integer large spin S via an Ising-type exchange interaction J and with the hopping terms $\lambda_{1(2)}$ (being $\lambda_2 = 0$ for this case) to a helical spin-texture chain hosted by an s -wave superconductor. (b) Side view of panel (a) wherein the QI-lead coupling Γ and Ising-type exchange interaction J for the spin-polarized tip and QI appear highlighted. (c) Pictorial scheme of panel (b), which effectively consists of a topological superconductor (TSC), where ϵ_M represents the overlap between the Majorana zero-modes (MZMs) γ_1 and γ_2 at edges, while the QI shows the MIQ γ_{MIQ} . The spatial distributions of the wave functions for the MZMs and QI are also illustrated. The factor $\frac{1}{4}$ in $\mathcal{G}_{\text{MIQ}}$ has correspondence to the $\frac{1}{4}$ from the volume for the sphere depicted to represent the quasiparticle γ_{MIQ} , in contrast to the ratio $\frac{1}{2}$ for the typical volume of the MZMs γ_1 and γ_2 . (d) Andreev bound state (ABS) regime, obtained from the effective model with $|\lambda_1| \sim |\lambda_2|$ [33]. (e) These MZMs mimic a delocalized fermionic site f , wherein ϵ_M plays the role of its energy level, while the QI has $2S+1$ levels ranging from $-J(S/2)$ to $+J(S/2)$. In this scenario, such quantum dots constitute a Kitaev dimer, i.e., with hopping t and pairing Δ of the p -wave Cooper pair split into the QI and f orbitals.

ence phenomenon [52, 53]. However, perfectly far apart MZMs are hypothetical objects, since they are reliable solely in infinite-size systems and in real experiments, the quantum wires are finite. As a result, these end MZMs within a finite length overlap with each other and inevitably, a fermionic mode with a finite energy emerges instead.

To overcome the aforementioned challenge, in this work, we find as route the fractionalization of ordinary MZMs, in particular, those found at a quantum impurity (QI) site coupled to one edge of a finite TSC in 1D. To this end, we should take into account the Ising exchange interaction between an integer large spin and such a QI. This setup corresponds to Figs. 1(a) and (b), and it contains the ordinary MZMs γ_1 and γ_2 placed at the edges of a short TSC wire. To better understand our findings, we propose to view the MZMs as sketched

in Fig. 1(c), where these objects appear symbolized by calottes (half-spheres). We clarify that the employment of such a pictorial representation for the MZMs aims to explain diagrammatically the electron fractionalization into them, as well as the MZM fractionalization itself here observed. These calottes belong to a delocalized sphere cut in half, with each part placed at the TSC edges. This cartoon is very useful and it has the purpose of emulating the nonlocal nature of the fermionic state composed by these MZMs, which are found spatially far apart. To best of our knowledge, the Majorana zero-frequency spectral weight, in particular for a QI coupled to an infinite TSC, is given by the unity when the leaking of the MZM γ_1 into a quantum dot occurs [4]. This unity corresponds to a calotte, which is a half-electron state that contributes to the conductance $\mathcal{G}_{\text{MZM}}(0) = \frac{e^2}{2h}$, as expected [3, 4]. Particularly for a finite TSC, we define as the system sweet spot [see Fig. 3(b)-I] a special configuration, in which a peculiar Ising exchange interaction allows us to observe a fractionalized MZM quasiparticle excitation γ_{MIQ} at the QI, namely, the called by us as Majorana-Ising-type quasiparticle (MIQ) excitation [Figs. 1(a) and (c)]. This quasiparticle excitation can be viewed as the half-calotte within the cartoon representation of the QI state [see also Fig. 1(c)]. Such a ratio symbolizes a novel MZM-type excitation in the presence of finite TSCs, in which technically speaking, it is identified by a Majorana zero-frequency spectral weight equals to half. Equivalently, the same amount corresponds to $\frac{1}{4}$ of the entire QI electronic state. In contrast, it leads to $\mathcal{G}_{\text{MIQ}}(0) = \frac{e^2}{4h}$ as it should be. Interestingly enough, solely in one of the Majorana densities of states (DOSs) of the QI, the MIQ becomes evident as a resonant mode localized at $\omega = 0$. Counterintuitively, the other Majorana DOS of the QI instead of exhibiting a resonant state, reveals a Majorana zero-frequency spectral weight with a valley, but presenting the same magnitude of the resonant Majorana fermion. In this manner, we can safely state that this novel MZM-type quasiparticle excitation, which for simplicity, we just call by MIQ from now on, is then found at the QI. In this situation, we demonstrate that the emergence of such a quasiparticle excitation yields a zero-bias local Andreev conductance entirely null, with only normal electronic contribution to the total conductance.

II. THE MODEL

The effective system Hamiltonian that corresponds to the proposed setup presented in Fig. 1(a) can be expressed

as:

$$\begin{aligned} \mathcal{H} = & \sum_{\alpha k \sigma} \varepsilon_{\alpha k} c_{\alpha k \sigma}^\dagger c_{\alpha k \sigma} + \sum_{\sigma} \varepsilon_{\sigma} d_{\sigma}^\dagger d_{\sigma} + i \varepsilon_M \gamma_1 \gamma_2 \\ & + \left(\frac{\Gamma}{2\pi\rho_0} \right)^{1/2} \sum_{\alpha k \sigma} (c_{\alpha k \sigma}^\dagger d_{\sigma} + \text{H.c.}) + J s^z S^z \\ & + \lambda_1 (d_{\uparrow} - d_{\uparrow}^\dagger) \gamma_1 + \lambda_2 (d_{\uparrow} + d_{\uparrow}^\dagger) \gamma_2, \end{aligned} \quad (1)$$

where the operator $c_{\alpha k \sigma}^\dagger (c_{\alpha k \sigma})$ describes the creation (annihilation) of an electron with momentum k , spin- z $\sigma = \pm 1$, energy $\varepsilon_{\alpha k} = \varepsilon_k - \mu_{\alpha}$ for the metallic lead $\alpha = [\text{Source}, \text{Drain}]$ in terms of the single-particle energy ε_k and chemical potential μ_{α} , while $d_{\sigma}^\dagger (d_{\sigma})$ stands for the electrons at the QI site in which ε_{σ} represents their energy levels per spin. To connect the QI to the metallic leads and a large spin S as well, we should consider the QI-lead coupling $\Gamma = 2\pi v^2 \rho_0$, which is determined by the QI-lead hopping term v and lead DOS ρ_0 , in parallel to the Ising-type exchange interaction J [Fig.1(b)]. This Ising Hamiltonian involves the components s^z and S^z of the QI ($s = 1/2$) and S , respectively, wherein the latter could be well-represented, within an experimental framework, by a spin-polarized tip [Ref.[54] and Figs.1(a)-(b)]. The emergence of MZMs at the TSC wire edges are accounted for γ_1 and γ_2 , with ε_M as the overlap parameter. Finally, λ_1 and λ_2 couple the spin-up channel of the QI to γ_1 and γ_2 , respectively [Figs.1(a) and (c)]. Additionally, for the sake of simplicity, we consider that the spin-down degree is decoupled from the TSC and obeys the single impurity Anderson model (SIAM)[55]. Thus, we assume that the spin component of the QI that couples to the Kitaev wire is $\sigma = +1$, which is, as can be viewed in Fig.1(a), the same spin direction assumed for the edges of the magnetic chain of adatoms. This means that the spin-flips of the QI electron injected into the TSC and vice-versa are prevented. Therefore, the spin-up degree of the QI is the unique to perceive the TSC. Different spin-textures on the TSC edge where γ_1 is found[56], which would allow the mixing of the spin degrees of freedom, will be addressed elsewhere and do not belong to the current analysis. Additionally, as we assume the intrinsic Zeeman splitting $\varepsilon_{\downarrow} - \varepsilon_{\uparrow} = V_Z$ of the magnetic chain as the largest energy scale, the spin-down has no influence in the phenomenon here reported, once the corresponding electronic occupation is empty. However, even with the present assumption, we are free to demonstrate that both these spin components become influenced by S and the TSC that mimics an effective quantum dot tunnel and Andreev-coupled to the QI [Fig.1(e),[57, 58]].

To this end, we call the attention that the Majorana and Ising terms of Eq.(1) should be conveniently rewritten to access the system underlying Physics: (i) the Ising term turns straightforwardly into

$$J s^z S^z = \frac{J}{2} \sum_{m \sigma} \sigma m d_{\sigma}^\dagger d_{\sigma} |m\rangle \langle m|, \quad (2)$$

due to the standard expansions $s^z = \frac{1}{2} \sum_{\sigma} \sigma d_{\sigma}^\dagger d_{\sigma}$ and

$S^z = \sum_m m |m\rangle \langle m|$ with $m = [-S, -S+1, \dots, S-1, S]$ for the QI and large spin, respectively. This means that each spin channel in the QI acquires a multi-level structure split into $2S+1$ energies ranging from $-J(S/2)$ to $+J(S/2)$. As a matter of fact, the TSC alters this feature quite a bit for the channel $\sigma = +1$; and (ii) it is imperative to evoke that the MZMs are made by the electron ($f^\dagger$) and hole (f) of a regular Dirac fermion delocalized over the TSC edges, which lead to $\gamma_1 = \frac{1}{\sqrt{2}}(f^\dagger + f)$ and $\gamma_2 = \frac{i}{\sqrt{2}}(f^\dagger - f)$. In this picture, ε_M plays the role of the energy level related to the electronic occupation $f^\dagger f$ and the QI is indeed hybridized with f , as mentioned earlier, via the hopping t and the superconducting pairing Δ . In summary, by considering the parameterization $\lambda_1 = (t+\Delta)/\sqrt{2}$ and $\lambda_2 = i(\Delta-t)/\sqrt{2}$ [Fig.1(a)], we simply find the Kitaev dimer composed by $d_{\uparrow}$ and f orbital sites[57, 58]:

$$\begin{aligned} & i \varepsilon_M \gamma_1 \gamma_2 + \varepsilon_{\uparrow} d_{\uparrow}^\dagger d_{\uparrow} + \lambda_1 (d_{\uparrow} - d_{\uparrow}^\dagger) \gamma_1 + \lambda_2 (d_{\uparrow} + d_{\uparrow}^\dagger) \gamma_2 \\ & = \varepsilon_M (f^\dagger f - \frac{1}{2}) + \varepsilon_{\uparrow} d_{\uparrow}^\dagger d_{\uparrow} + (t d_{\uparrow} f^\dagger + \Delta d_{\uparrow} f + \text{H.c.}). \end{aligned} \quad (3)$$

Similarly, the spin-up channel of the QI can be also decomposed in MZMs[4], which we label by γ_A and γ_B , i.e.,

$$d_{\uparrow} = \frac{1}{\sqrt{2}}(\gamma_A + i\gamma_B). \quad (4)$$

Based on Eq.(4), one can compute the Majorana zero-frequency spectral weights for γ_A and γ_B , respectively. These quantities reveal that in the poor man's Majorana regime ($J = 0$, $\Delta = t$ and $\varepsilon_M = \varepsilon_{\uparrow} = 0$)[57, 58] for the Kitaev dimer, that at the QI site, one spectral weight shows a unitary amplitude for a resonant zero-mode, while the other is completely null at zero-energy. It means that an isolated MZM is found at the QI. Analogously, such a feature is also observed in f [4, 32]. This results, according to Eq.(3) given by $i\sqrt{2}\lambda_1\gamma_B\gamma_1$, into two isolated MZMs spatially placed at $d_{\uparrow}$ and f orbital sites, namely, γ_A and γ_2 , respectively. Although f is already nonlocal and split over the TSC edges, it should be understood as an orbital site in the framework of the Kitaev dimer, thus γ_2 , within such a context, is placed there. For the trivial case ($\varepsilon_M \neq 0$), the two spectral weights for γ_A and γ_B attain to unity and then, two resonant zero-modes emerge at the QI site. Thus, Eq.(4) is extremely clarifying, once it points out the possibility of having within the QI, in the presence of ε_M and J , the isolation of the here proposed MIQ. Additionally, as one can notice, the spin down channel always shows the trivial case, due to its decoupling from the TSC. For completeness, the MZMs for $d_{\downarrow}$ we label by γ_C and γ_D . To conclude, we are aware that the QI could also be coupled to the s -wave platform of Fig.1(a) as in Ref.[51] by the term $\mathcal{H}_{s-QI} \sim -\Gamma_s (d_{\uparrow}^\dagger d_{\downarrow}^\dagger + \text{H.c.})$ [36, 51] in the limit $\Delta_{SC} \rightarrow \infty$ (infinite superconducting gap standard approximation), where Γ_s is the s -wave-QI coupling. Nevertheless, differently, we do not consider the on top geometry of Ref.[51]

and assumes intrinsic Zeeman splitting $\varepsilon_{\downarrow} - \varepsilon_{\uparrow} = V_Z$ of the magnetic chain extremely high, in order to rid off the spin-down component. As a result, we expect that both features suppress $\mathcal{H}_{s-QI}$ and let the exploration to elsewhere when V_Z is not found magnified.

III. QUANTUM TRANSPORT AND GREEN'S FUNCTIONS

In this section, our goal is the analytical evaluation of the total conductance through the QI device depicted in Figs.1(a)-(b). As a matter of fact, solely the spin-up channel contributes to the conductance, once the spin-down is energetically inaccessible as previously stated. As our goal is the transport determination around the energy of the MZM, only the bias-energy between source and drain leads $|eV| \ll \Delta_{SC} \rightarrow \infty$ (infinite superconducting gap standard approximation) is accounted for in the derivation of our conductance expression below [see Ref.[59] and Appendix B]. In the case of a grounded TSC, symmetric QI-lead couplings (Γ) independent of $\mu_{\text{Source}} - \mu_{\text{Drain}} = eV$, being $\mu_{\text{Source}} = -\mu_{\text{Drain}} = eV/2$, where e is the elemental charge and V the corresponding bias-voltage, the crossed Andreev reflection is suppressed and the conductance can be split into[59]

$$\mathcal{G}_{\text{Total}} = \mathcal{G}_{\text{ET}} + \mathcal{G}_{\text{LAR}}, \quad (5)$$

where ET and LAR stand for the electron tunneling and local Andreev reflection processes, respectively, with

$$\mathcal{G}_{\text{ET}}(eV) = \frac{e^2}{2h} [\tau_{\alpha\bar{\alpha}}^{\text{ET}}(eV/2) + \tau_{\alpha\bar{\alpha}}^{\text{ET}}(-eV/2)], \quad (6)$$

wherein $\alpha = \text{Source}$, $\bar{\alpha} = \text{Drain}$ and vice-versa, together with

$$\mathcal{G}_{\text{LAR}}(eV) = \frac{e^2}{2h} [\tau_{\alpha\alpha}^{\text{LAR}}(eV/2) + \tau_{\alpha\alpha}^{\text{LAR}}(-eV/2)], \quad (7)$$

in which the transmittances $\tau_{\alpha\bar{\alpha}}^{\text{ET}} = (2S + 1)\Gamma^2 |\langle\langle d_{\uparrow}; d_{\uparrow}^{\dagger} \rangle\rangle_{\omega}|^2$ and $\tau_{\alpha\alpha}^{\text{LAR}} = (2S + 1)\Gamma^2 |\langle\langle d_{\uparrow}^{\dagger}; d_{\uparrow}^{\dagger} \rangle\rangle_{\omega}|^2$ are expressed in terms of the frequency-dependent Green's functions (GFs) of type $\langle\langle A_{\sigma}; B_{\sigma} \rangle\rangle_{\omega} = \sum_m \langle\langle A_{\sigma}|m\rangle\langle m|; B_{\sigma} \rangle\rangle_{\omega}$ (details in the Appendix A), due to the presence of the large spin, in which the thermal average $\langle|m\rangle\langle m|\rangle = \frac{1}{2S+1}$ should be taken into account. Particularly, these GFs, are indeed the time Fourier transform (with $k_B = \hbar = 1$) of

$$\langle\langle A_{\sigma}; B_{\sigma} \rangle\rangle_{\omega} = \int \sum_m \langle\langle A_{\sigma}(t)|m(t)\rangle\langle m(t)|; B_{\sigma}(0) \rangle\rangle e^{i\omega^+ t} dt, \quad (8)$$

where $\omega^+ = \omega + i\eta^+$, with $\eta^+ \rightarrow 0$ and

$$\begin{aligned} \langle\langle A_{\sigma}(t)|m(t)\rangle\langle m(t)|; B_{\sigma}(0) \rangle\rangle &= -i\theta(t)\mathcal{Z}^{-1}\text{Tr}\{e^{-\mathcal{H}/T} \\ &\quad [A_{\sigma}(t)|m(t)\rangle\langle m(t)|, B_{\sigma}(0)]_+\} \end{aligned} \quad (9)$$

stands for the time-dependent GF following double-brackets Zubarev notation[60], wherein Tr gives the trace over Eq.(1) eigenstates, $\mathcal{Z}$ is the partition function and $[\dots]_+$ as the anticommutator.

In practice, the GFs should be determined via the standard equation-of-motion (EOM) approach[61], which in frequency domain, can be summarized as follows

$$\omega^+ \langle\langle A_{\sigma}; B_{\sigma} \rangle\rangle_{\omega} = \langle[A_{\sigma}, B_{\sigma}]_+\rangle + \langle\langle [A_{\sigma}, \mathcal{H}]; B_{\sigma} \rangle\rangle_{\omega}. \quad (10)$$

Additionally, Ref.[59] also ensures that the QI normalized DOS obeys the decomposition

$$\text{DOS}(\uparrow) = -\Gamma \text{Im} \langle\langle d_{\uparrow}; d_{\uparrow}^{\dagger} \rangle\rangle_{\omega} = \tau_{\alpha\bar{\alpha}}^{\text{ET}} + \tau_{\alpha\alpha}^{\text{LAR}}. \quad (11)$$

As Eq.(11) is bounded to unity, it describes the electronic overall transmittance through the QI decomposed into ET and LAR processes. Specially when it attains to its maximum value at zero energy, i.e., the $\text{DOS}(\uparrow)(0) = 1$ value gives the electronic zero-frequency spectral weight. In this case, the regular fermionic state of the QI is then made equally by the MZMs γ_A and γ_B . Equivalently, it means that the corresponding normalized DOSs for such quasiparticles localize Majorana states with the same spectral weights and as a result, the QI state is fully built by a pair of resonant MZMs. It gives rise to the conductance $\mathcal{G}_{\text{Total}}(0) = \frac{e^2}{h}$. Interestingly enough for $\text{DOS}(\uparrow)(0) = 1/2$, an isolated ordinary MZM is found at the QI site and the zero-bias conductance is characterized by the hallmark $\mathcal{G}_{\text{Total}}(0) = \frac{e^2}{2h}$ [3, 4]. Such a case corresponds to an ideal infinite superconducting wire. However, there is a regime in which the value $\text{DOS}(\uparrow)(0) = 1/2$ is still present for a finite wire and due to the Ising interaction between the large spin and the QI, the observation of the conductance $\mathcal{G}_{\text{Total}}(0) = \frac{e^2}{2h}$ is ensured. This emerges from the novel excitation that we introduce as the MIQ, in particular, by driving the system into the sweet spot for the exchange interaction J , namely, $J = J_h$. In the latter, the index “h” stands for the “half-fermion” special condition of a MZM, which is produced by imposing $\text{DOS}(\uparrow)(0) = 1/2$, from where we extract J_h for a given S [see Fig.3 b)-I].

Therefore, in order to reveal the aforementioned Physics about the system conductance, we should begin evaluating Eq.(6) for the electron tunneling process. Thus, the GF $\langle\langle d_{\uparrow}; d_{\uparrow}^{\dagger} \rangle\rangle_{\omega}$ should be found via the EOM method, which gives

$$\langle\langle d_{\uparrow}; d_{\uparrow}^{\dagger} \rangle\rangle_{\omega} = \frac{1}{2S+1} \sum_m \frac{1}{\omega^+ - \varepsilon_{\uparrow} - \frac{Jm}{2} + i\Gamma - \Sigma_{\text{MFs}}^+}, \quad (12)$$

where $\Sigma_{\text{MFs}}^+ = K_+ + (2t\Delta)^2 K_{\text{MFs}} \tilde{K}_m$ represents the self-energy correction due to the couplings of the QI with the TSC and the large spin S . This also depends on the following defined quantities

$$K_{\text{MFs}} = \frac{\omega^+}{\omega^2 - \varepsilon_M^2 + 2i\omega\eta^+ - (\eta^+)^2}, \quad (13)$$

$$K_{\pm} = \frac{\omega^+(\Delta^2 + t^2) \pm \varepsilon_M(t^2 - \Delta^2)}{\omega^2 - \varepsilon_M^2 + 2i\omega\eta^+ - (\eta^+)^2} \quad (14)$$

and

$$\tilde{K}_m = \frac{K_{\text{MFS}}}{\omega^+ + \varepsilon_{\uparrow} + \frac{J_m}{2} + i\Gamma - K_-}. \quad (15)$$

Concerning the LAR, the conductance of Eq.(7) needs the evaluation of the anomalous GF $\langle\langle d_{\uparrow}^{\dagger}; d_{\uparrow}^{\dagger} \rangle\rangle_{\omega}$ instead. After performing the EOM approach, it gives rise to

$$\langle\langle d_{\uparrow}^{\dagger}; d_{\uparrow}^{\dagger} \rangle\rangle_{\omega} = -\frac{1}{2S+1} \sum_m \frac{2t\Delta K_m}{\omega^+ + \varepsilon_{\uparrow} + \frac{J_m}{2} + i\Gamma - \Sigma_{\text{MFS}}^{-m}}, \quad (16)$$

with $\Sigma_{\text{MFS}}^{-m} = K_- + (2t\Delta)^2 K_{\text{MFS}} K_m$ and

$$K_m = \frac{K_{\text{MFS}}}{\omega^+ - \varepsilon_{\uparrow} - \frac{J_m}{2} + i\Gamma - K_+}. \quad (17)$$

However, if we want to know about the possibility of isolating MZMs in the QI, the DOSs for γ_A and γ_B should be found in order to examine the emergence of resonant states. To this end, we invert Eq.(4) for γ_A and γ_B , namely, $\gamma_A = (d_{\uparrow}^{\dagger} + d_{\uparrow})/\sqrt{2}$ and $\gamma_B = i(d_{\uparrow}^{\dagger} - d_{\uparrow})/\sqrt{2}$, and we calculate the GFs $\langle\langle \gamma_A; \gamma_A \rangle\rangle_{\omega}$ and $\langle\langle \gamma_B; \gamma_B \rangle\rangle_{\omega}$. Consequently,

$$\begin{aligned} \langle\langle \gamma_j; \gamma_j \rangle\rangle_{\omega} &= \frac{1}{2} [\langle\langle d_{\uparrow}; d_{\uparrow}^{\dagger} \rangle\rangle_{\omega} + \langle\langle d_{\uparrow}^{\dagger}; d_{\uparrow} \rangle\rangle_{\omega} \\ &\quad + \epsilon (\langle\langle d_{\uparrow}^{\dagger}; d_{\uparrow}^{\dagger} \rangle\rangle_{\omega} + \langle\langle d_{\uparrow}; d_{\uparrow} \rangle\rangle_{\omega})], \end{aligned} \quad (18)$$

where $j = (A, B)$ corresponds to $\epsilon = (+1, -1)$, respectively. Physically speaking, the sign reversal in ϵ can lead to distinct quantum interference phenomena, in particular between those encoded by the normal GFs ($\langle\langle d_{\uparrow}; d_{\uparrow}^{\dagger} \rangle\rangle_{\omega}$ and $\langle\langle d_{\uparrow}^{\dagger}; d_{\uparrow} \rangle\rangle_{\omega}$) and the corresponding superconducting ($\langle\langle d_{\uparrow}^{\dagger}; d_{\uparrow}^{\dagger} \rangle\rangle_{\omega}$ and $\langle\langle d_{\uparrow}; d_{\uparrow} \rangle\rangle_{\omega}$). To reveal such interference processes, we need just to find the GFs $\langle\langle d_{\uparrow}^{\dagger}; d_{\uparrow} \rangle\rangle_{\omega}$ and $\langle\langle d_{\uparrow}; d_{\uparrow}^{\dagger} \rangle\rangle_{\omega}$ to close the evaluation of $\langle\langle \gamma_A; \gamma_A \rangle\rangle_{\omega}$ and $\langle\langle \gamma_B; \gamma_B \rangle\rangle_{\omega}$. By applying the EOM method, we conclude that

$$\langle\langle d_{\uparrow}^{\dagger}; d_{\uparrow} \rangle\rangle_{\omega} = \frac{1}{2S+1} \sum_m \frac{1}{\omega^+ + \varepsilon_{\uparrow} + \frac{J_m}{2} + i\Gamma - \Sigma_{\text{MFS}}^{-m}} \quad (19)$$

and

$$\langle\langle d_{\uparrow}; d_{\uparrow}^{\dagger} \rangle\rangle_{\omega} = -\frac{1}{2S+1} \sum_m \frac{2\Delta t \tilde{K}_m}{\omega^+ - \varepsilon_{\uparrow} - \frac{J_m}{2} + i\Gamma - \Sigma_{\text{MFS}}^{+m}}. \quad (20)$$

Naturally, we define the normalized DOSs for γ_A and γ_B such as

$$\text{DOS}(\uparrow)[\gamma_j] = -\Gamma \text{Im} \langle\langle \gamma_j; \gamma_j \rangle\rangle_{\omega}. \quad (21)$$

This formula elucidates that when the quantity $\text{DOS}(\uparrow)[\gamma_j](0) = -\Gamma \text{Im} \langle\langle \gamma_j; \gamma_j \rangle\rangle_{\omega}(0) = 1$ is fulfilled, it can be recognized as the maximum Majorana quasiparticle transmittance or its corresponding zero-frequency spectral weight.

Henceforward, we focus the attention on the case $\varepsilon_{\uparrow} = 0$ (grounded SC). We perceive by inspecting Eqs.(12) and (19), that Eq.(11) becomes also $\text{DOS}(\uparrow) = -\Gamma \text{Im} \langle\langle d_{\uparrow}^{\dagger}; d_{\uparrow} \rangle\rangle_{\omega}$. Additionally, $-\Gamma \text{Im} \langle\langle d_{\uparrow}^{\dagger}; d_{\uparrow}^{\dagger} \rangle\rangle_{\omega} = -\Gamma \text{Im} \langle\langle d_{\uparrow}; d_{\uparrow} \rangle\rangle_{\omega}$. This in combination with Eqs.(18) and (21) allow us to establish that

$$\text{DOS}(\uparrow) = \frac{1}{2} (\text{DOS}(\uparrow)[\gamma_A] + \text{DOS}(\uparrow)[\gamma_B]). \quad (22)$$

Consequently, by taking into account this finding together with Eqs.(5), (6), (7) and (11), we conclude the providential equality as follows

$$\mathcal{G}_{\text{Total}} = \mathcal{G}_{\gamma_A} + \mathcal{G}_{\gamma_B}, \quad (23)$$

where

$$\mathcal{G}_{\gamma_j}(\text{eV}) = \frac{e^2}{4h} [\text{DOS}(\uparrow)[\gamma_j](\text{eV}/2) + \text{DOS}(\uparrow)[\gamma_j](-\text{eV}/2)] \quad (24)$$

stands for the conductance contribution arising from the quasiparticle γ_j within the QI.

We highlight that Eq.(23) introduces an alternative perspective concerning the underlying Physics of the conductance in Eq.(5): the ET and LAR quantum transport mechanisms are revealed as the net effect of two Majorana quasiparticle conductances, namely, the corresponding contributions arising from γ_A and γ_B , respectively. In this context, our main findings hold for the constraint $J = J_h$ fulfilled, thus characterizing the system sweet spot to produce the MIQ. This regime consists of the maximum Majorana quasiparticle transmittance $\text{DOS}(\uparrow)[\gamma_j](0) = 1$, surprisingly, fractionalized and split into $\text{DOS}(\uparrow)[\gamma_A](0) = 1/2$ and $\text{DOS}(\uparrow)[\gamma_B](0) = 1/2$. Despite such equipartition, the electronic transmittance is still given by $\text{DOS}(\uparrow)(0) = 1/2$ [see Fig.3 b)-I] and according to Eq.(24), it ensures $\mathcal{G}_{\gamma_A}(0) = \frac{e^2}{4h}$ and $\mathcal{G}_{\gamma_B}(0) = \frac{e^2}{4h}$. However, counterintuitively, solely $\mathcal{G}_{\gamma_B}(0)$ contains a MZM in the common sense, i.e., a resonant state, while $\mathcal{G}_{\gamma_A}(0)$ shows a dip instead, but with the same magnitude of the peak in γ_B . This is the reason why we call the contribution $\mathcal{G}_{\gamma_B}(0) = \frac{e^2}{4h}$ by $\mathcal{G}_{\text{MIQ}}(0)$, in attention to the emergent MIQ. This is the unique MZM-type resonant state that appears in the system, due to the interplay between the topological superconductivity and the Ising Hamiltonian. In this case, Eqs.(5) and (23) ensure that when the MIQ emerges, $\mathcal{G}_{\gamma_B}(0)$ exhibits a maximum and $\mathcal{G}_{\gamma_A}(0)$ shows a minimum, in such a way that only $\mathcal{G}_{\text{ET}}(0)$ enters into $\mathcal{G}_{\text{Total}}(0) = \frac{e^2}{2h}$. It means that the LAR process is found entirely suppressed within this regime. The complete analysis here summarized will be discussed in the next section.

IV. RESULTS

In the entire numerical analysis of Sec.A, we keep constant $\varepsilon_{\uparrow} = 0$ (grounded SC), $\lambda_1 = 2.12\Gamma$ ($\Delta = t$) and perform variations in the parameters ε_M , S and J . Partially for Sec.B, we assume $|\lambda_1| \sim |\lambda_2|$ [$\Delta \neq 0, t \rightarrow 0$] from Eq.(1) [Eq.(3)] to analyze the ABSs regime within the framework of the effective model[33]. We should remember that $\mu_{\text{Source}} - \mu_{\text{Drain}} = eV$ represents the bias-energy between source and drain leads, with the choice $\mu_{\text{Source}} = -\mu_{\text{Drain}} = eV/2$ in our transport calculations.

A. Majorana-Ising-type quasiparticle (MIQ) excitation

In Fig.2 we present, for the QI of Fig.1, the total conductance of Eq.(5) as a function of the bias-voltage eV/Γ . Particularly in Fig.2(a) the ideal case is considered, i.e., the TSC wire is perfectly infinite ($\varepsilon_M = 0$) and the large spin is found turned-off ($S = 0$). This case is well-known, being characterized by the ZBP in the conductance given by $\mathcal{G}_{\text{Total}}(0) = \frac{e^2}{2h}$ [3, 4]. Interestingly enough, this ZBP in the conductance represents the isolated MZM γ_1 originally attached to one edge of the TSC wire, which leaks towards the QI site in the form of the MZM γ_A . The MZM leakage from the TSC edge into the QI is then characterized by the $\text{DOS}(\uparrow)[\gamma_A](0) = 1$ and $\text{DOS}(\uparrow)[\gamma_B](0) = 0$. We will provide extra details concerning this issue in the discussion of the inset a)-I of Fig.3(a). In the other hand, the satellite peaks in Fig.2(a) are the aftermath of the splitting arising from the condition $i\sqrt{2}\lambda_1\gamma_B\gamma_1$ given by Eq.(3) for the *poor man's Majoranas* regime of the system[57, 58]. Additionally, we have made explicit via Eq.(5) that the ET and LAR processes compose the total conductance. Thus, such a feature can be viewed in Fig.2(b), where we notice, in particular, for the ZBP conductance that, the ET and LAR split equally. Here we propose that it is still achievable to obtain $\mathcal{G}_{\text{Total}}(0) = \frac{e^2}{2h}$ for a finite TSC wire and to perform also the isolation of a Majorana quasiparticle at the QI site. In our setup, such an excitation rises, in particular, dressed by the Ising interaction. To this end, an integer large spin S should be accounted for and be coupled to the QI with a special value in the exchange interaction J . Thus, by evaluating $J = J_h$, the amplitude $\mathcal{G}_{\text{Total}}(0) = \frac{e^2}{2h}$ [Eq.(23)] finally becomes restored. However, we will verify that such a configuration corresponds to isolate a peculiar MZM, namely γ_B , with a resonant peak characterized by the spectral weight $\text{DOS}(\uparrow)[\gamma_B](0) = 1/2$ [Eq.(21)], while for γ_A we have the same amplitude, i.e., $\text{DOS}(\uparrow)[\gamma_A](0) = 1/2$, but with a dip instead.

Now, we consider the presence of a large spin S . Figs.2(c) and (d) show the total conductance in the presence of $S = 3$ and $J_h = 1.335\Gamma$ [see inset b)-I of Fig.3(b)] for a finite TSC with $\varepsilon_M = \Gamma$. The ZBP

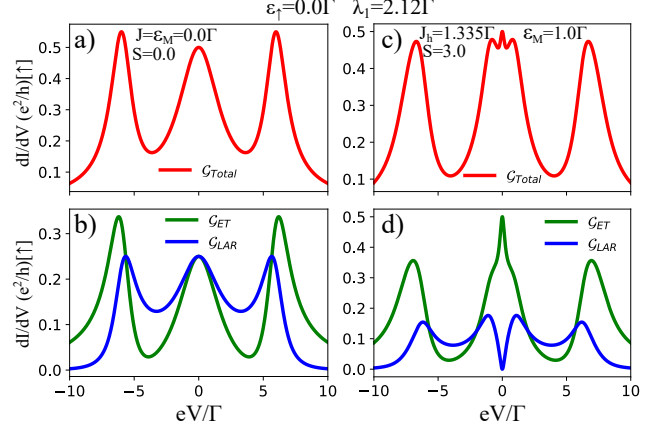


Figure 2. (Color online) (a) Total differential conductance $\mathcal{G}_{\text{Total}}$ [Eq.(5)] versus the source-drain bias-voltage eV in units of the QI-lead coupling Γ with isolated MZMs γ_1 and γ_2 ($\varepsilon_M = 0$) in the absence of a spin-polarized tip ($S = 0$). As aftermath, a zero-bias peak (ZBP) emerges with amplitude $\mathcal{G}_{\text{Total}}(0) = \frac{e^2}{2h}$ and characterizes the leaking of the MZM γ_1 from the TSC wire edge [Fig.1(c)] into the QI as γ_A [inset a)-I of Fig.3(a) and Refs.[3, 4]. (b) The ZBP conductance can be split into finite contributions from the electron tunneling (ET) and local Andreev reflection (LAR) processes [Eq.(5)], namely, $\mathcal{G}_{\text{ET}}(0)$ and $\mathcal{G}_{\text{LAR}}(0)$, respectively. This corresponds to the ideal case of an infinite TSC wire, wherein these processes compete on equal footing. (c) In the presence of a tip with $S = 3$ and exchange coupling at the sweet spot $J = J_h = 1.335\Gamma$ [inset b)-I of Fig.3(b)] for a finite wire ($\varepsilon_M = 1\Gamma$), the amplitude $\mathcal{G}_{\text{Total}}(0) = \frac{e^2}{2h}$ is still observed and denotes the existence of a MIQ γ_{MIQ} within the QI, but with related differential conductance $\mathcal{G}_{\text{MIQ}}(0) = \frac{e^2}{4h}$ [Fig.3(c) and Eqs.(23)-(24)]. (d) In the regime of (c), $\mathcal{G}_{\text{LAR}}(0)$ is completely quenched and solely the term $\mathcal{G}_{\text{ET}}(0)$ contributes to the ZBP.

conductance in Fig.2(c) is $\mathcal{G}_{\text{Total}}(0) = \frac{e^2}{2h}$ as expected, but the decomposition into ET and LAR channels described in Fig.2(d) reveals a striking result: solely ET survives, while LAR is completely suppressed at zero-bias. Below we will verify that the LAR suppression corresponds to a quasiparticle localization in the DOS for γ_B , which leads to $\text{DOS}(\uparrow)[\gamma_B](0) = 1/2$. Thus, according to Eq.(24), such a finite DOS contributes to a conductance $\mathcal{G}_{\gamma_B}(0) = \mathcal{G}_{\text{MIQ}}(0) = \frac{e^2}{4h}$, where we define the MIQ $\gamma_B \equiv \gamma_{\text{MIQ}}$.

In order to understand the emergence of the MIQ, we begin with the trivial case in Fig.3(a): the central panel discriminates the electronic $\text{DOS}(\uparrow)$ into the corresponding DOSs for γ_A and γ_B [Eq.(21)] with $S = 0$ and $\varepsilon_M = \Gamma$. This case is regarded as trivial, once we verify that in both the DOSs γ_A and γ_B resonant states pinned at zero-energy $\omega = 0$ are present. Schematically, the QI fermionic state can be imagined as a sphere formed by two MZMs depicted by two calottes. This is the manner we outline pictorially the two zero-energy resonant states, the so-called MZMs in the DOSs γ_A and γ_B . This sketch can be found in the upper-right inset of Fig.3(a), in which

each calotte symbolizes the “half-fermionic” character of the MZM. Equivalently, a calotte occupies the half-volume of the sphere and as it corresponds to a MZM, it can be surely characterized by $\text{DOS}(\uparrow)[\gamma_j](0) = 1$. As aftermath, according to Eqs.(22)-(24), these two MZMs lead to the zero-bias conductance peak $\mathcal{G}_{\text{Total}}(0) = \frac{e^2}{h}$. Concerning the satellite peaks in the $\text{DOS}(\uparrow)[\gamma_B]$, they occur due to the overlap between the MZMs γ_B and γ_1 . In the other hand, the inset panel a)-II of Fig.3(a) shows the spin-down channel, which is the one decoupled from the TSC. To analyze it on the same footing as the spin-up channel, we assume artificially $\varepsilon_\downarrow = 0$ and verifies that both the MZMs γ_C and γ_D , which constitute this spin sector of the QI, are then identified exactly by degenerate resonant states. The evaluation of the DOSs for the spin-down sector just employs the GFs for the spin-up sector, but it disregards the superconducting terms. As none of these MZMs overlap with γ_1 , a full superposition of the lineshapes for these MZMs manifests in the profiles of the DOSs γ_C and γ_D . Therefore, satellite peaks do not emerge. Now, let us go back to discuss the spin-up channel. We should pay particular attention to the case $\varepsilon_M = 0$ depicted in the inset panel a)-I of Fig.3(a), which corresponds to the nonoverlapped situation between γ_1 and γ_2 . This scenario is the ideal one and it contains the pillars for the conductance behavior of Fig.2(a). Notice that γ_B overlaps with γ_1 leading to satellite peaks in $\text{DOS}(\uparrow)[\gamma_B]$ and $\text{DOS}(\uparrow)[\gamma_B](0) = 0$, while γ_A is found isolated and localized as a well-defined resonant zero-mode with spectral weight $\text{DOS}(\uparrow)[\gamma_A](0) = 1$. Thereafter, $\mathcal{G}_{\text{Total}}(0) = \mathcal{G}_{\gamma_A}(0) = \frac{e^2}{2h}$. This case is well-known in literature [3, 4] and points out that the MZM γ_A contributes to the conductance as a resonant state in contrast to γ_B , which shows a gap in $\text{DOS}(\uparrow)[\gamma_B]$ around zero-bias. This latter prevents a finite conductance, i.e., $\mathcal{G}_{\gamma_B}(0) = 0$. Below, we will see that by turning-on the exchange J for a given S , the spectral profiles for the $\text{DOS}(\uparrow)[\gamma_A]$ and $\text{DOS}(\uparrow)[\gamma_B]$ will exhibit a multi-level structure. Additionally, these densities will be responsible, according to Eq.(24), by a nonquantized $\mathcal{G}_{\text{Total}}(0) \neq \frac{e^2}{h}$ in Eq.(23). In the situation of arbitrary J , the contributions to $\mathcal{G}_{\text{Total}}(0) \neq 0$ will not arise from well-defined resonant zero-mode states in $\text{DOS}(\uparrow)[\gamma_A]$ and $\text{DOS}(\uparrow)[\gamma_B]$. The Majorana fermion localization within the QI as a resonant zero-mode state will only occur for the sweet spot $J = J_h$.

Fig.3(b) treats the presence of a large spin coupled to the QI for $\varepsilon_M = \Gamma$. As we can notice, the Ising interaction $J = 5\Gamma$ for $S = 3$ clearly affects the spectral profiles of $\text{DOS}(\uparrow)[\gamma_A]$ and $\text{DOS}(\uparrow)[\gamma_B]$. Basically, it introduces a multi-level structure for the satellite peaks and modifies drastically the MZM localization around the zero-bias. Surprisingly, the $\text{DOS}(\uparrow)[\gamma_A]$ presents a valley (dip) at zero-energy and a quasi-resonant MZM rises in $\text{DOS}(\uparrow)[\gamma_B]$. As a matter of fact, the latter cannot be considered a well-defined resonant MZM: its spectral weight is not exactly an integer or semi-integer number, and

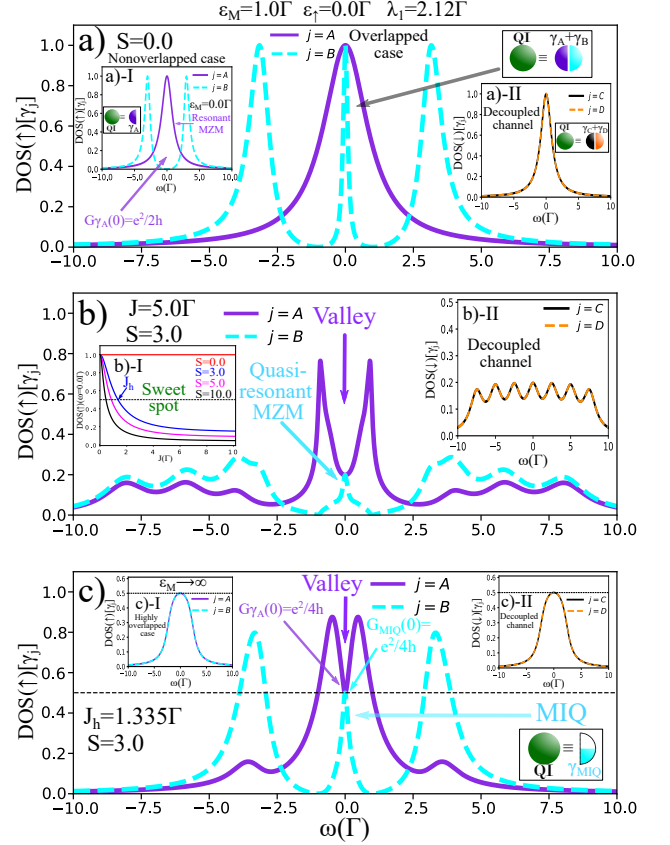


Figure 3. (Color online) (a) The central panel shows the frequency dependence of the normalized densities of states (DOSs) for the MZMs γ_A and γ_B [Eq.(21)] for the spin-up channel within the QI by assuming the spin-polarized tip absent and the MZMs γ_1 and γ_2 overlapped ($\varepsilon_M = 1\Gamma$) in the TSC. In each DOS we find a resonant MZM, which corresponds to a “half-fermionic” state of the QI depicted as the green sphere in the upper-right inset. This sphere has inner MZMs represented by calottes to denote the half-fermion nature of the MZM. In the nonoverlapped situation, only the calotte γ_A prevails [inset a)-I]. It leads to $\mathcal{G}_{\text{Total}}(0) = \mathcal{G}_{\gamma_A}(0) = \frac{e^2}{2h}$ in Fig.2(a) [Eqs.(23)-(24)]. For the spin-down channel, which is decoupled from the TSC, the MZMs γ_C and γ_D within the QI stay paired permanently [inset a)-II]. (b) In the presence of $S = 3$ and $J = 5\Gamma$ for $\varepsilon_M = 1\Gamma$ the DOS for γ_A changes drastically exhibiting a valley at $\omega = 0$ instead of a peak, while for γ_B the zero-mode is not well defined. To restore the ZBP $\mathcal{G}_{\text{Total}}(0) = \frac{e^2}{2h}$ we should choose the right J for a given S , i.e., the sweet spot $J = J_h$ [panel b)-I] for the QI DOS of Eq.(22) imposing $\text{DOS}(\uparrow)(0) = 1/2$. In the spin-down channel, the γ_C and γ_D DOSs are degenerate with a $2S + 1$ multi-level structure [panel b)-II]. (c) The choice $J = J_h = 1.335\Gamma$ for $S = 3$ completely defines the valley and peak for the DOSs γ_A and γ_B , respectively, where in the latter we introduce $\gamma_B \equiv \gamma_{\text{MIQ}}$ as the Majorana-Ising quasi-particle, once the peak clearly represents the unique MZM isolated in the system. It is characterized by a ZBP given by $\mathcal{G}_{\text{MIQ}}(0) = \frac{e^2}{4h}$ pictorially illustrated by the half-calotte in the lower-right inset for the green sphere representing the QI fermionic state. However, $\mathcal{G}_{\text{Total}}(0) = \mathcal{G}_{\gamma_A}(0) + \mathcal{G}_{\text{MIQ}}(0) = \frac{e^2}{2h}$.

the lineshape broadening does not obey a *lorentzian-like* form. The lineshapes of such spectral densities are then distinct, but counterintuitively, their zero-bias values coincide, i.e., $\text{DOS}(\uparrow)[\gamma_A](0) = \text{DOS}(\uparrow)[\gamma_B](0)$. As the spin-up sector of the QI is the one coupled to the TSC, the spectral profiles in the $\text{DOS}(\uparrow)[\gamma_A]$ and $\text{DOS}(\uparrow)[\gamma_B]$ do not follow strictly the standard angular momentum theory for the Zeeman splitting [Eq.(2)]. Usually, this theory ensures that for an integer S , $2S$ symmetrically displaced levels around the corresponding at $\omega = \varepsilon_\uparrow = 0$ should emerge. Here, indeed we observe a mirror-symmetric set with S energy bands below and above the zero-bias, respectively, where nearby peculiar spectral structures rise. We reveal that the profiles differ significantly in this range, as aftermath of the nontrivial interplay between the TSC and Ising exchange term. In Figs.4(d)-(f) we will see that the manifestation of this effect lies within a region comprised by *cone-like walls* spanned by ω and ε_M in the DOSs of the system. Within the cone, the Zeeman splitting becomes unusual and the energy spacing between the levels is simultaneously governed by J and ε_M . Besides, solely the spin-down channel shows standard Zeeman splitting, once it does not perceive the TSC. This can be verified in the inset panel b)-II of Fig.3(b), where the DOSs for γ_C and γ_D , as expected, present the ordinary $2S+1$ multi-level structure ensured by Eq.(2). We highlight that upon decreasing the exchange parameter J , the restoration of the conductance $\mathcal{G}_{\text{Total}}(0) = \frac{e^2}{2h}$ can be still allowed. Thus, we should remember that such a conductance arises from the fulfillment of the condition $\text{DOS}(\uparrow)(0) = 1/2$. Particularly in the inset panel b)-I of Fig.3(b), we show exactly the points where this happens by considering several values of S and $\varepsilon_M \neq 0$. Particularly for $S = 3$, this sweet spot occurs for $J = J_h = 1.335\Gamma$ and its dependence on ε_M is revealed as very weak according to our numerical calculations (not shown). It means that $J = J_h = 1.335\Gamma$ still keeps the value $\text{DOS}(\uparrow)(0) = 1/2$ while ε_M does not exceed very much Γ ($\varepsilon_M \gg \Gamma$). Experimentally speaking, J can be tuned by changing the tip-QI vertical distance. Thus for $\varepsilon_M \neq 0$, $\mathcal{G}_{\text{Total}}(0)$ drops from $\frac{e^2}{h}$ to $\frac{e^2}{2h}$ when $J = J_h$. Hence, at the sweet spot, if one knows previously the spin S of the tip, J_h can be extracted from Fig.3 b)-I or vice-versa.

In Fig.3(c) we present the case $J = J_h = 1.335\Gamma$ that leads to our main finding: a localization of a resonant state at zero-energy in $\text{DOS}(\uparrow)[\gamma_B]$, with spectral weight $\text{DOS}(\uparrow)[\gamma_B](0) = 1/2$. The latter amplitude points out that the ordinary MZM now is fractionalized and the value $\text{DOS}(\uparrow)[\gamma_B](0) = 1$ is not present anymore. This fractionalized MZM, the called MIQ by us, then leads to a conductance $\mathcal{G}_{\gamma_B}(0) = \mathcal{G}_{\text{MIQ}}(0) = \frac{e^2}{4h}$ as ensured by Eq.(24). The value $\text{DOS}(\uparrow)[\gamma_B](0) = 1/2$ can be pictorially viewed by the half-calotte found in the lower-right inset of Fig.3(c), which symbolizes the MZM fractionalization within the QI state. Nevertheless, to complete the total conductance $\mathcal{G}_{\text{Total}}(0) = \frac{e^2}{2h}$, the zero-bias value for $\text{DOS}(\uparrow)[\gamma_A](0)$ should coincide, i.e.,

$\text{DOS}(\uparrow)[\gamma_A](0) = 1/2$ and as aftermath, $\mathcal{G}_{\gamma_A}(0) = \frac{e^2}{4h}$ as well. Here we emphasize that in $\text{DOS}(\uparrow)[\gamma_A](0)$ a quantum destructive interference manifests and a resonant state does not rise at zero-bias. Moreover, it is capital to clarify the underlying mechanism to produce the MIQ: the key idea is the decrease of J , thus forcing the merge of the $2S$ side bands (satellite peaks) of the system towards the zero-energy, where a resonant level is pinned. As a result, this sum of amplitudes for the satellite peaks interferes constructively at zero-energy giving rise to $\text{DOS}(\uparrow)(0) = 1/2$ for $J = J_h$. Further, our findings do not depend on the sign of J and in case of a semi-integer large spin, the multi-level structure is even and a zero-energy is absent in the spectrum. In this manner, the MIQ cannot be excited. Concerning the inset panels c)-I and c)-II of Fig.3(c), we verify that for $\varepsilon_M \gg \Gamma$ (or $\varepsilon_M \rightarrow \infty$) the DOSs for the Majorana fermions are degenerate. For extremely short TSC wires ($\varepsilon_M \rightarrow \infty$), the energy level ε_M for the orbital f [Eq.(3)] is highly off resonance the QI energy $\varepsilon_\uparrow = 0$, thus making the QI and the TSC to decouple from each other. Thus, the spin-up channel behaves as the corresponding spin-down, which is the one permanently decoupled from the TSC. This implies that the MIQ cannot be seen for very short wires.

Fig.4 summarizes our findings exhibiting color maps of Eqs.(11) and (21) for the electronic and Majorana DOSs, respectively and spanned by ω and ε_M . Panels (a)-(c) describe the case $S = 0$, which is characterized by $\text{DOS}(\uparrow)(0) = 1$ and $\text{DOS}(\uparrow)[\gamma_A](0) = \text{DOS}(\uparrow)[\gamma_B](0) = 1$. This corresponds to the trivial regime where two MZMs localize around zero-bias and appear at the QI site. Such a characteristic lies on the zero-bias peaks and appears as horizontal lines in the representation of panels (a)-(c) for any finite value of ε_M . As we can see, the satellite peaks in (a) arise from (c). By turning-on the Ising interaction with $S = 3$ and $J = 5\Gamma$, the spectral profiles of the DOSs acquire distinct patterns: the satellite peaks obey approximately the standard angular momentum theory for the Zeeman splitting, thus exhibiting $2S$ split sidebands. In this situation, the linear dependence on the exchange parameter J is lacking. Besides, the central regions of panels (a)-(c) are converted into the domains delimited by *cone-like walls* as those found in (d)-(f). While these walls persist up to a threshold in ε_M (not marked in the figure), a sophisticated interplay between the TSC and the Ising interaction rules the Physics of the system and allows the possibility of the MIQ existence. Notice that for $\varepsilon_M > \Gamma$, a $2S+1$ multi-level central structure finally becomes resolved. It is worth mentioning that for $\varepsilon_M = \Gamma$, the line cuts in Fig.4 given by the vertical dashed lines, then correspond to the cases discussed in detail in Fig.3. We would like to mention that the choice $\varepsilon_M = \Gamma$ corresponds to a strong limit, just to better resolve our findings. However, while ε_M stays within the aforementioned *cone-like walls*, the effect persists. In panels (e) and (f) we notice the rising of the valley and the quasi-resonant MZM spectral struc-

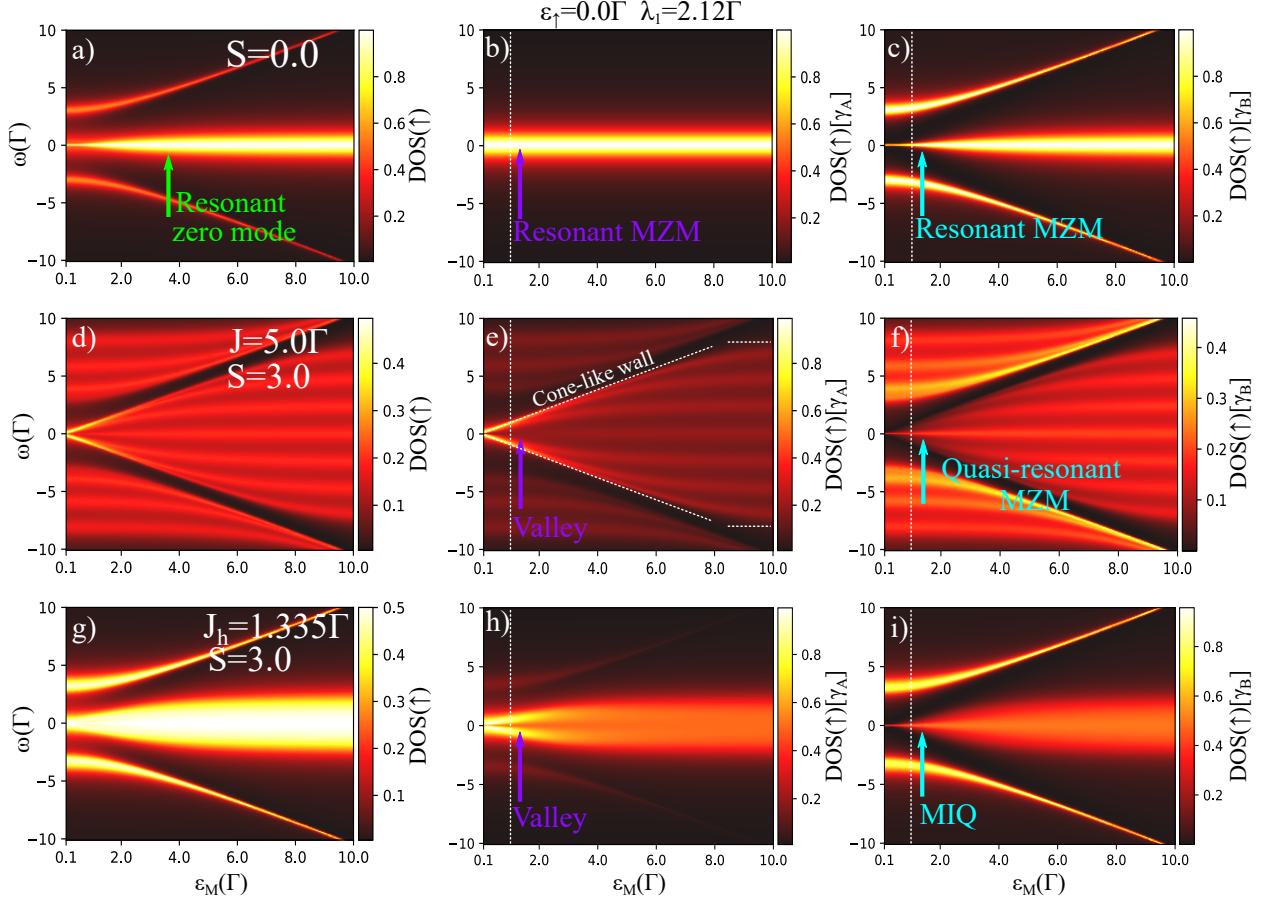


Figure 4. (Color online) Color maps of Eqs.(11) and (21) for the QI, γ_A and γ_B DOSs, respectively, spanned by the frequency ω and ϵ_M : (a) In the case $S = 0$, the ZBP in the DOS($\uparrow$) arises from the individual ZBPs found in DOS($\uparrow$)[γ_A] [panel(b)] and DOS($\uparrow$)[γ_B] [panel(c)], due to the MZMs γ_A and γ_B that act as the building-blocks of the QI state $\epsilon_\uparrow = 0$ [Eq.(22)]. They reveal that the system does not contain isolated MZMs and that the overlapped γ_1 and γ_2 split the zero-mode energy state leading to the upper and lower arcs in panels (a) and (c). Panels (d)-(f) reveal the influence of $S = 3$ and $J = 5\Gamma$ on the QI, where we can clearly see a $2S + 1$ multi-level structure centered at $\omega = 0$. The upper and lower arcs, distinctly, show $2S$ levels each. The central region of (e) has a valley-type structure in contrast to that for (f), which points out a quasi-resonant MZM. In both the cases, the $2S + 1$ multi-level structure is delimited by cone-like walls up to a threshold in ϵ_M (not indicated), where above it the DOS($\uparrow$)[γ_A] and DOS($\uparrow$)[γ_B] exhibit a zero-mode with the lines of the walls parallel to each other. For this situation, the TSC plays no role and the MZMs γ_A and γ_B stay paired as in (a)-(c). Panels (g)-(i) hold for the sweet spot $J = J_h = 1.335\Gamma$, where we have the zero-frequency valley and peak well-resolved in the DOS($\uparrow$)[γ_A] and DOS($\uparrow$)[γ_B], respectively. In the latter, the MIQ rises as aftermath of the partial merge of the $2S + 1$ multi-level structure centered at $\omega = 0$ upon decreasing the coupling J . We call the attention that the vertical lines represent slice cuts of the cases profoundly explored in Figs.2 and 3.

tures, respectively upon increasing ϵ_M . However, much above the threshold in ϵ_M , the linear spacing in J for the Zeeman splitting is restored and this situation is that delimited by the marked horizontal dashed lines. Finally, panels (g)-(i) show the merge of the multi-level structure in the sweet spot $J = J_h = 1.335\Gamma$ leading to the emergence of the MIQ in the Majorana channel γ_B , while the valley continues in the channel γ_A . Therefore, within the cone-like walls domain, the sector γ_B of Majorana fermions for the QI makes explicit a constructive interference process at zero-bias, while the corresponding in γ_A displays a destructive behavior. In this regime, the conductance $\mathcal{G}_{\text{LAR}}(0)$ becomes fully quenched and just

$\mathcal{G}_{\text{ET}}(0)$ contributes to $\mathcal{G}_{\text{Total}}(0) = \frac{e^2}{2h}$ [Fig.2(d)].

B. Poor man's Majoranas, parity qubit and ABSs regime

In this section, we clarify that the MIQ excitation can be classified as a *poor man's Majorana* [57, 58] and to demonstrate such, the analysis of the DOSs for the MZMs of Eq.(3) placed at the Kitaev dimer right edge is performed. To accomplish this goal, we employ pertinent GFs from the Appendix C. Additionally, we discuss the possibility of having a MIQ excitation-based par-

ity qubit for quantum computing purposes[57] and the ABSs regime within the effective model of Eq.(1)[33]. To this end, let us focus again on the left edge of the Kitaev dimer, i.e., the QI. This system part description is found in central panel of Fig.3(a) ($\varepsilon_M = \Gamma$) and its inset a)-I ($\varepsilon_M = 0$), which account for the QI operator $d_\uparrow$, where the MZMs γ_A and γ_B reside [Eq.(4)]. Particularly, these panels show two resonant and single MZMs, respectively, while in Fig.5(a), a resonant MZM appears permanently in the DOS $(-1/\pi)\text{Im}\langle\gamma_2; \gamma_2\rangle_\omega$ (not normalized, once leads are lacking at this side) for γ_2 in both the situations, thus describing the MZM placed at the TSC right edge. Such a characteristic is entirely understood within the theoretical framework for the Kitaev dimer described in Ref.[57]. The latter points out that systems based on Eq.(3) for QIs tunnel and Andreev-coupled, which in our case are given by the $d_\uparrow$ and f orbital sites, could contain the so-called *poor man's Majoranas*. These MZMs, in particular, cannot be considered topologically protected as true MZMs, and emerge at the M. Leijnse *et al* sweet spot[57], when the following set of parameters is obeyed: $J = 0$, $\Delta = t$ and $\varepsilon_M = \varepsilon_\uparrow = 0$. This scenario can be observed in the inset panels a)-I of Figs.3 and 5, which reveal resonant MZMs, namely, the *poor man's Majoranas*, with one placed at left and the other at right of the Kitaev dimer. This statement holds, since the spectral weights are given by the $\text{DOS}(\uparrow)[\gamma_A](0) = 1$ and $\text{DOS}(\uparrow)[\gamma_B](0) = 0$ for the QI [inset a)-I of Fig.3(a)], while we have $\text{DOS}[\gamma_1](0) = 0$ and $\text{DOS}[\gamma_2](0) \neq 0$ for the Kitaev dimer right edge, as depicted in the inset of Fig.5(a). For the aforementioned case, the nonlocal fermion $\eta = (\gamma_A - i\gamma_2)/\sqrt{2}$ can be made via the linear combination between the resonant MZMs γ_2 and γ_A localized at right and left of the dimer, respectively[57]. In this manner, the fermion parity, which is given by the electronic occupation of $\eta^\dagger\eta$, becomes a feasible quantity for quantum computing[57]. For the resonant MZMs γ_A and γ_B at left depicted in central panel of Fig.3(a) and the corresponding in Fig.5(a), i.e., the situation off the M. Leijnse *et al* sweet spot with $\varepsilon_M = \Gamma$, the fragility of these *poor man's Majoranas* becomes evident. In such a case, the spectral weights $\text{DOS}(\uparrow)[\gamma_A](0) = 1$ and $\text{DOS}(\uparrow)[\gamma_B](0) = 1$ occur simultaneously at the QI. Thus, according to Ref.[57], the zero-mode dip in the DOS $(-1/\pi)\text{Im}\langle\gamma_1; \gamma_1\rangle_\omega$ represents the spill of the MZM γ_1 from the f orbital site over the QI, being characterized by the $\text{DOS}(\uparrow)[\gamma_B](0) = 1$. As after-math, these two resonant MZMs inevitably introduce an ambiguous definition for the nonlocal parity qubit, i.e., it could be $\eta = (\gamma_A - i\gamma_2)/\sqrt{2}$ or $\eta = (\gamma_B - i\gamma_2)/\sqrt{2}$. In this way, the parity qubit becomes not well-defined and its employment compromised, as expected, for quantum computing.

With this in mind, we back to our sweet spot in Fig.3, where the Ising term J_h , by considering $\varepsilon_M = \Gamma$, siphons off the $\text{DOS}(\uparrow)[\gamma_A](0) = 1$ [Fig.3(a)] from resonant profile towards one antiresonant with $\text{DOS}(\uparrow)[\gamma_A](0) = 1/2$ [Fig.3(c)], while it keeps the $\text{DOS}(\uparrow)[\gamma_B = \gamma_{\text{MIQ}}](0) =$

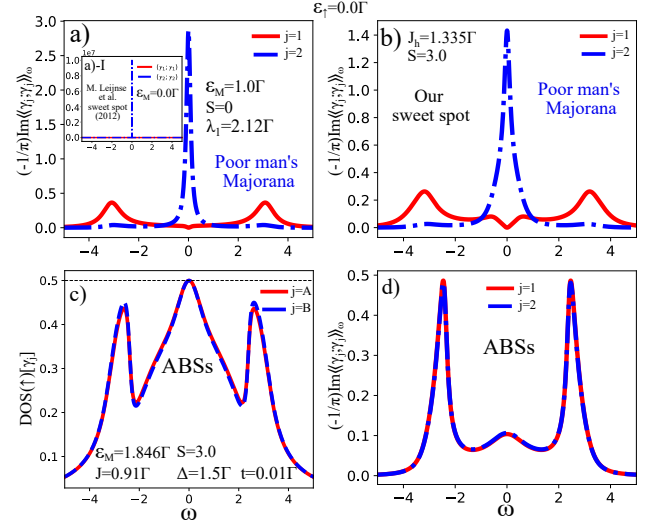


Figure 5. (Color online) Panels (a) and (b) show M. Leijnse *et al*[57] and our sweet spots, respectively for *poor man's Majoranas*. The Andreev bound states (ABSs) regime of Refs.[33, 34] appear depicted in panels (c) and (d). Additionally, fractionalization of zero-modes also occurs in the latter.

$1/2$ [Fig.3(c)] resonant after such a deviation from the value $\text{DOS}(\uparrow)[\gamma_B](0) = 1$ [Fig.3(a)]. As the MZM given by γ_{MIQ} exhibits resonant character and its partner γ_A is of antiresonant-type, it means that the QI does not host exactly one MZM. It is an indication that a MZM is spilled over the QI from the f orbital site, where the $\text{DOS}[\gamma_1](0) = 0$ and the resonant $\text{DOS}[\gamma_2](0) \neq 0$ still persist, as can be seen in Fig.5(b). Thus, such features reinforce that the MIQ excitation obeys the properties of the poor man's Majorana[57]. Let us remember that in panels a)-I from Figs.3 and 5, the left and right resonant MZMs were linearly combined to build η when $\varepsilon_M = 0$. However, an extrapolation to $\eta = (\gamma_{\text{MIQ}} - i\gamma_2)/\sqrt{2}$ for $\varepsilon_M \neq 0$ instead, despite being $\gamma_B = \gamma_{\text{MIQ}}$ resonant and γ_A not, deserves further investigation, once Ref.[57] does not cover such a limit. We let the advances on this particular parity qubit issue to better exploration elsewhere, since they do not belong to the scope of our current research. We call attention that our main findings consist of showing one way of realizing the fractionalization of MZMs, in particular, via the Ising coupling to a QI site.

Still concerning the nature of the fractionalized spectral weight peak given by $\text{DOS}(\uparrow)[\gamma_{\text{MIQ}}](0) = 1/2$, we attribute its origin to several modes that added up result into a half-integer contribution. Indeed, each mode, as we know, due to the QI-leads coupling, becomes a band centered at the mode in the absence of the leads. As the separation between the modes (centers of these bands) depends directly on the Ising coupling J , by decreasing to $J = J_h$ (our sweet spot), it favors the partial merge of the $2S + 1$ odd number of bands at zero-energy, where there is an accumulation point. This is naturally imposed by the choice of an integer S . Consequently,

we find the peak $\text{DOS}(\uparrow)[\gamma_{\text{MIQ}}](0) = 1/2$ and the dip $\text{DOS}(\uparrow)[\gamma_A](0) = 1/2$, when we fix $\text{DOS}(\uparrow)(0) = 1/2$ in Eq.(22).

In summary, as demonstrated by us, the MIQ excitation (the resonant one) and γ_A (the corresponding partner antiresonant) at the system left, together with γ_2 at right, are *poor man's Majoranas*, since they obey their properties of partially protection (not topological) introduced by Ref.[57]. It is worth mentioning that *poor man's Majoranas* were recently verified in the experiment of Ref.[58] and in our case, the *poor man's Majoranas* observed at the QI show fractionalized characteristic, due to the Ising coupling. At the M. Leijnse *et al* sweet spot[57], the Ising term plays no role and we still have $\text{DOS}(\uparrow)(0) = 1/2$, but with the $\text{DOS}(\uparrow)[\gamma_B](0) = 0$ and a peak in the $\text{DOS}(\uparrow)[\gamma_A](0) = 1$, thus reflecting not fractionalized MZMs. In both the sweet spots, it is capital to note that we have always $\mathcal{G}_{\text{Total}}(0) = \frac{e^2}{2h}$, once we adopt the right side of Eq.(4) as the basis for the quasiparticle excitations of the electron at the QI [Eq.(11)]. This basis is convenient to evaluate the system quantum transport and elucidates if just one MZM (M. Leijnse *et al* sweet spot) or half of each from the MZM couple of quasiparticle excitations at the QI (our sweet spot), is really contributing to $\mathcal{G}_{\text{Total}}(0) = \frac{e^2}{2h}$.

Figs.5(c) and (d) discuss the ABSs regime, which can be captured by imposing $|\lambda_1| \sim |\lambda_2|$ [$\Delta \neq 0$, $t \rightarrow 0$] in Eq.(1) [Eq.(3)], as pointed out by Ref.[33]. It is worth mentioning that such a scenario corresponds to place the MZMs γ_1 and γ_2 practically at same TSC edge [see Fig.1(d)], with model parameters marked in Fig.5(c), from where we highlight $\Delta = 1.5\Gamma$ and $t = 0.01\Gamma$. Thus, it leads to a conductance $\mathcal{G}_{\text{Total}}(0) = \frac{e^2}{2h}$, which is purely from electron tunneling, but counterintuitively, assisted by Andreev reflection. It means that although $\mathcal{G}_{\text{LAR}}(\text{eV}) \rightarrow 0$ through the QI flanked by the leads [Eqs.(7), (16) and (20)], the Kitaev dimer, indeed still admits Andreev reflection, in particular, between the $d_\uparrow$ and f orbitals given by the terms $\Delta d_\uparrow f + \text{H.c.}$ [Eq.(3),[57]], which then build the quasiparticle electronic state at the QI. As Eqs.(23) and (24) also determine $\mathcal{G}_{\text{Total}}(0) = \frac{e^2}{2h}$, in Fig.5(c), we evaluate then the DOSs $\text{DOS}(\uparrow)[\gamma_j] = -\Gamma \text{Im}\langle\langle\gamma_j; \gamma_j\rangle\rangle_\omega$ [Eq.(21)], which strongly depend only on the GFs $\langle\langle d_\uparrow; d_\uparrow^\dagger \rangle\rangle_\omega$ and $\langle\langle d_\uparrow^\dagger; d_\uparrow \rangle\rangle_\omega$ [Eq.(18)], since $\langle\langle d_\uparrow; d_\uparrow \rangle\rangle_\omega = \langle\langle d_\uparrow^\dagger; d_\uparrow^\dagger \rangle\rangle_\omega \rightarrow 0$ [Eqs.(16) and (20)] in the ABS regime. By looking at Eqs.(A1) and (A2) in the Appendix A, we verify that $\langle\langle d_\uparrow; d_\uparrow^\dagger \rangle\rangle_\omega$ and $\langle\langle d_\uparrow^\dagger; d_\uparrow \rangle\rangle_\omega$ have a dependence on $\Delta\langle\langle f^\dagger|m\rangle\langle m|; d_\uparrow^\dagger \rangle\rangle_\omega$ and $\Delta\langle\langle f|m\rangle\langle m|; d_\uparrow \rangle\rangle_\omega$, which are modulated by the SC pairing Δ and GFs associated to $\Delta d_\uparrow f + \text{H.c.}$ for the Andreev process. Such features establish the Andreev reflection between the QI and f , while $\mathcal{G}_{\text{LAR}}(\text{eV}) \rightarrow 0$ is evaluated at the interface QI-leads. Additionally, we should highlight that similar analysis in observing the ABSs regime, in particular, within the effective model of Eq.(1) but without the Ising term, was already performed

by some of us via the analogous Eq.(20) of Ref.[34] and now, we extend it to the current Hamiltonian. As consequences, Fig.5(c) also exhibits the DOSs siphon off to $1/2$ for γ_A and γ_B , which distinct from Figs.5(a) and (b) with $\Delta = t$, are identically resonant. In Fig.5(d), a pair of ABSs manifests too. To conclude, $\mathcal{G}_{\text{Total}}(0) = \frac{e^2}{2h}$ could be reproduced by both the *poor man's Majoranas* and ABSs regimes.

V. CONCLUSIONS

We found that the fractionalization of regular MZMs becomes a feasible task once an integer large spin S is exchange coupled to a quantum impurity, in particular when it acts as the new edge of a finite TSC in 1D. A counterintuitive regime arises due to a sweet value for the Ising coupling, which is capable of localizing a fractionalized MZM. We introduce such an excitation as the called Majorana-Ising-type quasiparticle (MIQ). As aftermath, we report the emergence of one MZM with the maximum spectral weight reduced by half and exhibiting resonant character. In contrast, the other MZM mode in the QI does not localize around zero-energy, but shows the same spectral weight of the resonant MZM via an antiresonant profile. Interestingly enough, due to the localization of the MIQ, half of the quantum conductance is made essentially by the normal electronic contribution, while that from the Andreev reflection is totally lacking between the QI and leads. This behavior differs from that observed in perfectly infinite TSC wires, in which one MZM localizes at QI site with maximum spectral weight given by unit and with electronic and Andreev conductances equally split at zero-bias. Therefore, our proposal points out a manner to induce, within a more realistic perspective from an experimental point of view, a quantum state at the edge of a short TSC in 1D. Additionally, our MIQ is demonstrated to be a *poor man's Majorana*[57, 58].

VI. ACKNOWLEDGMENTS

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Appendix A: Green's functions for the system left side

As the GFs in the presence of the large spin obey the notation $\langle\langle A_\sigma; B_\sigma \rangle\rangle_\omega = \sum_m \langle\langle A_\sigma | m \rangle\langle m |; B_\sigma \rangle\rangle_\omega$ [60], here we make explicit the details in the EOM approach to find the elements of type $\langle\langle A_\sigma | m \rangle\langle m |; B_\sigma \rangle\rangle_\omega$. In what follows, we have

$$\begin{aligned} & (\omega^+ - \varepsilon_\uparrow - \frac{Jm}{2} + i\Gamma) \langle\langle d_\uparrow | m \rangle\langle m |; d_\uparrow^\dagger \rangle\rangle_\omega \\ &= \frac{1}{2S+1} - t \langle\langle f | m \rangle\langle m |; d_\uparrow^\dagger \rangle\rangle_\omega - \Delta \langle\langle f^\dagger | m \rangle\langle m |; d_\uparrow^\dagger \rangle\rangle_\omega, \end{aligned} \quad (\text{A1})$$

$$\begin{aligned} & (\omega^+ + \varepsilon_\uparrow + \frac{Jm}{2} + i\Gamma) \langle\langle d_\uparrow^\dagger | m \rangle\langle m |; d_\uparrow \rangle\rangle_\omega \\ &= \frac{1}{2S+1} + t \langle\langle f^\dagger | m \rangle\langle m |; d_\uparrow \rangle\rangle_\omega + \Delta \langle\langle f | m \rangle\langle m |; d_\uparrow \rangle\rangle_\omega, \end{aligned} \quad (\text{A2})$$

the other two terms are given by

$$\begin{aligned} & (\omega^+ + \varepsilon_\uparrow + \frac{Jm}{2} + i\Gamma) \langle\langle d_\uparrow^\dagger | m \rangle\langle m |; d_\uparrow^\dagger \rangle\rangle_\omega \\ &= t \langle\langle f^\dagger | m \rangle\langle m |; d_\uparrow^\dagger \rangle\rangle_\omega + \Delta \langle\langle f | m \rangle\langle m |; d_\uparrow^\dagger \rangle\rangle_\omega \end{aligned} \quad (\text{A3})$$

and

$$\begin{aligned} & (\omega^+ - \varepsilon_\uparrow - \frac{Jm}{2} + i\Gamma) \langle\langle d_\uparrow | m \rangle\langle m |; d_\uparrow \rangle\rangle_\omega \\ &= -t \langle\langle f | m \rangle\langle m |; d_\uparrow \rangle\rangle_\omega - \Delta \langle\langle f^\dagger | m \rangle\langle m |; d_\uparrow \rangle\rangle_\omega \end{aligned} \quad (\text{A4})$$

And finally the last two GFs associated with the f site is

$$\begin{aligned} \langle\langle f | m \rangle\langle m |; d_\uparrow \rangle\rangle_\omega &= \frac{-t}{(\omega^+ - \varepsilon_M)} \langle\langle d_\uparrow | m \rangle\langle m |; d_\uparrow \rangle\rangle_\omega \\ &+ \frac{\Delta}{(\omega^+ - \varepsilon_M)} \langle\langle d_\uparrow^\dagger | m \rangle\langle m |; d_\uparrow \rangle\rangle_\omega \end{aligned} \quad (\text{A5})$$

and

$$\begin{aligned} \langle\langle f^\dagger | m \rangle\langle m |; d_\uparrow \rangle\rangle_\omega &= \frac{t}{(\omega^+ + \varepsilon_M)} \langle\langle d_\uparrow^\dagger | m \rangle\langle m |; d_\uparrow \rangle\rangle_\omega \\ &- \frac{\Delta}{(\omega^+ + \varepsilon_M)} \langle\langle d_\uparrow | m \rangle\langle m |; d_\uparrow \rangle\rangle_\omega. \end{aligned} \quad (\text{A6})$$

With this group of GFs we can determine the complete description of the QI.

Appendix B: Quantum transport formalism

Based on the quantum transport Keldysh formalism of Ref.[59], we wrap up here a summary of steps in deriving

Eqs.(6), (7) and (11), which assumes the subgap regime $|eV| \ll \Delta_{\text{SC}} \rightarrow \infty$ (infinite superconducting gap standard approximation) and wide-band limit characterized by an electron-hole symmetry in the QI-leads coupling, which is given by Γ [see the main text below Eq.(1)]. As a result, we have as the total current I_α at the metallic lead α the following

$$I_\alpha = I_\alpha^{\text{ET}} + I_\alpha^{\text{LAR}} + I_\alpha^{\text{CAR}}, \quad (\text{B1})$$

where

$$I_\alpha^{\text{ET}} = \frac{e}{h} \int d\varepsilon \tau_{\alpha\bar{\alpha}}^{\text{ET}}(\varepsilon) [f_\alpha^e(\varepsilon) - f_{\bar{\alpha}}^e(\varepsilon)], \quad (\text{B2})$$

$$I_\alpha^{\text{CAR}} = \frac{e}{h} \int d\varepsilon \tau_{\alpha\bar{\alpha}}^{\text{CAR}}(\varepsilon) [f_\alpha^e(\varepsilon) - f_{\bar{\alpha}}^h(\varepsilon)] \quad (\text{B3})$$

and

$$I_\alpha^{\text{LAR}} = \frac{e}{h} \int d\varepsilon \tau_{\alpha\bar{\alpha}}^{\text{LAR}}(\varepsilon) [f_\alpha^e(\varepsilon) - f_{\bar{\alpha}}^h(\varepsilon)], \quad (\text{B4})$$

where I_α^{ET} and I_α^{CAR} refer to the currents for the electron tunneling (ET) and crossed Andreev reflection (CAR) between the QI and the lead α , but with occupation probabilities of an electron $f_\alpha^e(\varepsilon)$ and hole $f_{\bar{\alpha}}^h(\varepsilon)$ states at lead $\bar{\alpha}$, respectively, where $f_\alpha^j(\varepsilon)$ stands for the Fermi distribution at lead α and $j = e(h)$ for the electron (hole) quasiparticle. For the local Andreev reflection (LAR) I_α^{LAR} , the hole emission is into the same terminal α , once it depends on $f_\alpha^h(\varepsilon)$.

As the total current should conserve, the Kirchhoff's law holds $I_\alpha + I_{\bar{\alpha}} + I_S = 0$. Additionally, the following assumptions are performed: $\mu_{\text{Source}} = -\mu_{\text{Drain}} = eV/2$ and the TSC is supposed to be grounded (null chemical potential $\mu_{\text{SC}} = 0$). The former implies in $f_\alpha^e(\varepsilon) = f_{\bar{\alpha}}^h(\varepsilon)$ and consequently $I_\alpha^{\text{CAR}} = 0$ from Eq.(B3), while the latter gives $I_S = 0$ and finally $I_\alpha = -I_{\bar{\alpha}}$. It means that the current only changes the sign from terminal α to $\bar{\alpha}$, being the conductance $\mathcal{G}_{\text{Total}}$ lead independent:

$$\mathcal{G}_{\text{Total}} = \frac{dI_\alpha}{dV} = \frac{dI_\alpha^{\text{ET}}}{dV} + \frac{dI_\alpha^{\text{LAR}}}{dV} = \mathcal{G}_{\text{ET}} + \mathcal{G}_{\text{LAR}}, \quad (\text{B5})$$

with

$$\begin{aligned} \frac{dI_\alpha^{\text{ET}}}{dV} &= \frac{e^2}{2h} \frac{1}{T} \int d\varepsilon \tau_{\alpha\bar{\alpha}}^{\text{ET}}(\varepsilon) \{f_\alpha^e(\varepsilon)[1 - f_\alpha^e(\varepsilon)] \\ &+ f_{\bar{\alpha}}^e(\varepsilon)[1 - f_{\bar{\alpha}}^e(\varepsilon)]\}, \end{aligned} \quad (\text{B6})$$

and

$$\begin{aligned} \frac{dI_\alpha^{\text{LAR}}}{dV} &= \frac{e^2}{2h} \frac{1}{T} \int d\varepsilon \tau_{\alpha\alpha}^{\text{LAR}}(\varepsilon) \{f_\alpha^e(\varepsilon)[1 - f_\alpha^e(\varepsilon)] \\ &+ f_\alpha^e(\varepsilon)[1 - f_\alpha^e(\varepsilon)]\}, \end{aligned} \quad (\text{B7})$$

where we employed the identity $f_\alpha^e(\varepsilon) = f_{\bar{\alpha}}^h(\varepsilon)$ again and

$$\frac{\partial f_{\alpha(\bar{\alpha})}^e(\varepsilon)}{\partial V} = \pm \frac{e}{2T} f_{\alpha(\bar{\alpha})}^e(\varepsilon) [1 - f_{\alpha(\bar{\alpha})}^e(\varepsilon)], \quad (\text{B8})$$

with $k_B = 1$, $f_{\alpha}^e(\varepsilon) = f(\varepsilon - eV/2)$, $f_{\bar{\alpha}}^e(\varepsilon) = f(\varepsilon + eV/2)$ and $f(x) = 1/(1 + e^{x/T})$.

As $\frac{1}{T} f_{\alpha(\bar{\alpha})}^e(\varepsilon) [1 - f_{\alpha(\bar{\alpha})}^e(\varepsilon)] = \left(-\frac{\partial f_{\alpha(\bar{\alpha})}^e(\varepsilon)}{\partial \varepsilon} \right) \rightarrow \delta(\varepsilon \mp eV/2)$ when $T \rightarrow 0\text{K}$, then we deduce Eqs.(6) and (7). To conclude, we should remember that the Keldysh formalism of Ref.[59] also ensures

$$I_{\alpha} = \frac{e}{h} \int d\varepsilon (-\Gamma \text{Im} \langle \langle d_{\uparrow}^{\dagger}; d_{\uparrow}^{\dagger} \rangle \rangle_{\omega}) [f_{\alpha}^e(\varepsilon) - f_{\bar{\alpha}}^e(\varepsilon)]. \quad (\text{B9})$$

Therefore, by comparing Eqs.(B9) and (B1), together with Eqs.(B2) and (B4), we finally determine Eq.(11).

Appendix C: Green's functions for the system right side

Here we show the GFs for the f orbital site and the MZMs γ_1 and γ_2 of the Kitaev dimer right side [Eq.(3)]. These quantities are important for Fig.5 and make explicit the *poor man's Majoranas*[57, 58] and ABSs[33] regimes in our system. As we know that $\gamma_1 = \frac{1}{\sqrt{2}}(f^{\dagger} + f)$ and $\gamma_2 = \frac{i}{\sqrt{2}}(f^{\dagger} - f)$, we naturally find the GF

$$\begin{aligned} \langle \langle \gamma_j; \gamma_j \rangle \rangle_{\omega} &= \frac{1}{2} [\langle \langle f; f^{\dagger} \rangle \rangle_{\omega} + \langle \langle f^{\dagger}; f \rangle \rangle_{\omega} \\ &+ \epsilon (\langle \langle f^{\dagger}; f^{\dagger} \rangle \rangle_{\omega} + \langle \langle f; f \rangle \rangle_{\omega})], \quad (\text{C1}) \end{aligned}$$

where $j = (1, 2)$ corresponds to $\epsilon = (+1, -1)$, respectively. By applying Eq.(10) for the EOM approach, we obtain

$$\langle \langle f; f^{\dagger} \rangle \rangle_{\omega} = \frac{1}{(2S+1)} \sum_m \frac{1}{(\omega^+ - \varepsilon_M - \Sigma_{+M})}, \quad (\text{C2})$$

$$\langle \langle f^{\dagger}; f \rangle \rangle_{\omega} = \frac{1}{(2S+1)} \sum_m \frac{1}{(\omega^+ + \varepsilon_M - \Sigma_{-M})}, \quad (\text{C3})$$

$$\langle \langle f^{\dagger}; f^{\dagger} \rangle \rangle_{\omega} = \frac{1}{(2S+1)} \sum_m \frac{2\Delta t K_{-M}}{(\omega^+ + \varepsilon_M - \Sigma_{-M})} \quad (\text{C4})$$

and

$$\langle \langle f; f \rangle \rangle_{\omega} = \frac{1}{(2S+1)} \sum_m \frac{2\Delta t K_{+M}}{(\omega^+ - \varepsilon_M - \Sigma_{+M})}. \quad (\text{C5})$$

with $\Sigma_{\pm M} = K_C^{\pm} + (2\Delta t)^2 K_D K_{\pm M}$ being the self-energy due to the interaction of the f site with the QI, which can be expressed in terms of the defined quantities

$$K_{+M} = \frac{K_D}{(\omega^+ + \varepsilon_M - K_C^-)}, \quad (\text{C6})$$

$$K_{-M} = \frac{K_D}{(\omega^+ - \varepsilon_M - K_C^+)}, \quad (\text{C7})$$

$$K_D = \frac{(\omega + i\eta^+) + i\Gamma}{(\omega + i\Gamma + i\eta^+)^2 - \varepsilon_{\uparrow}^2 - Jm[\varepsilon_{\uparrow} + \frac{Jm}{4}]}, \quad (\text{C8})$$

and

$$\begin{aligned} K_C^{\pm} &= \left[\frac{(\omega + i\eta^+) (t^2 + \Delta^2) \pm \varepsilon_{\uparrow} (t^2 - \Delta^2)}{(\omega + i\Gamma + i\eta^+)^2 - \varepsilon_{\uparrow}^2 - Jm[\varepsilon_{\uparrow} + \frac{Jm}{4}]} \right] \\ &+ \left[\frac{\pm \frac{Jm}{2} (t^2 - \Delta^2) + i\Gamma (t^2 + \Delta^2)}{(\omega + i\Gamma + i\eta^+)^2 - \varepsilon_{\uparrow}^2 - Jm[\varepsilon_{\uparrow} + \frac{Jm}{4}]} \right] \quad (\text{C9}) \end{aligned}$$

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