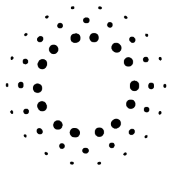

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Variational Method for the Wigner Functional Approach to Quantum Field Theory

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"You alone are the LORD. You made the heavens, even the highest heavens, and all their starry host, the earth and all that is on it, the seas and all that is in them. You give life to everything, and the multitudes of heaven worship you"

Nehemiah 9:6, *New International Version Bible*

Resumo

Construímos um formalismo variacional para calcular funcionais de Wigner em teoria quântica de campos através da generalização de um método desenvolvido na mecânica estatística não-relativística. O funcional de Wigner que usamos é uma generalização da função de Wigner usual em mecânica quântica, na qual amplitudes de campo e seus momentos conjugados são as variáveis dinâmicas do espaço de fase. O formalismo não perturbativo nos permite calcular sistematicamente correções à tradicional aproximação de campo médio para os funcionais de Wigner. Para desenvolver o formalismo, empregamos uma teoria de campo escalar com autointerações quárticas. Implementamos um exercício numérico para explorar alguns aspectos do formalismo e calculamos a função de correlação de dois pontos e a segunda entropia de Rényi.

Palavras Chaves: Teoria Quântica de Campos; Espaço de Fase; Função de Wigner.

Áreas do conhecimento: Física; Física de Partículas e Campos.

Abstract

We constructed a variational formalism to compute Wigner functionals in quantum field theory by generalizing a method developed in nonrelativistic statistical mechanics. The Wigner functional we use is a generalization of the standard Wigner function in quantum mechanics, in which field amplitudes and their conjugate momenta are the phase space dynamical variables. The nonpertubative formalism allows us to compute corrections to the traditional mean-field approximation for the Wigner functional. We used a scalar field theory with quartic self-interactions to set up the formalism. We performed a numerical exercise to explore some features of the formalism, and computed the two-point correlation function and the second Rényi entropy.

Key Words: Quantum Field Theory; Phase Space; Wigner Function.

Knowledge areas: Physics; Physics of Particles and Fields.

Contents

Chapter 1

Introduction

The phase space representation of classical physics dynamics is omnipresent since the late 1800's [1]. Wigner extended such a representation to quantum systems [2]. Wigner's main objective was to introduce quantum corrections to statistical mechanics using phase space dynamical variables. Nowadays, the quantum phase space quantization, also known as Moyal quantization or deformation quantization, is is an alternative, autonomous and logically concise, formulation of quantum mechanics [3, 4, 5]. One computes observables neither with operators and wave functions in Hilbert space nor with classical trajectories in a Feynman path integral; instead, one integrates c-numbers weighted by Wigner distribution functions. The similarity with statistical mechanics is, however, not complete since Wigner functions are not necessarily positive everywhere in phase space and hence are called "quasi-distribution" functions. Negativity of a Wigner function signals nonclassical features of the corresponding quantum state. Among the most striking nonclassical features is quantum entanglement, the quintessential quantum property. In recent years, negativity of the Wigner function has been recognized as a resource for continuous-variable quantum information processing and transmission [6].

The quantum phase space representation arises naturally from the Hamiltonian formulation of quantum dynamics. Due to the intrinsic lack of explicit Lorentz covariance of a Hamiltonian formulation, many authors, including Wigner [7], deemed the representation inappropriate for relativistic many-particle quantum systems. The skepticism was nevertheless unwarranted, as lack of explicit covariance does not obstruct a phase space representation when the entire formalism is grounded on a quantum field theory (QFT) framework [8, 9, 10, 11, 12, 13, 14, 15, 16, 17]. There are basically two conceptually distinct formulations of Wigner functions in QFT. The most commonly used employs field operators to define a covariant Wigner operator [18], whose expectation value with respect to a density operator is the covariant Wigner function [19, 9]. For one-particle states, such a Wigner functional reduces in the nonrelativistic limit to the standard quantum

mechanical Wigner function. This formulation is well suited to treat problems associated with the quark-gluon plasma in heavy-ion collisions; very recent studies include those in Refs. [20, 21, 22, 23, 24]. A different construction involves a natural generalization of the standard Wigner function, in that fields and their conjugate momenta are the phase space dynamical variables, instead of particle coordinates and momenta [11]; the Wigner functional is a functional of the fields and conjugate momenta. A similar formalism was constructed in Ref. [12]. As its nonrelativistic counterpart, the Wigner functional is not explicitly covariant since it is based on the Hamiltonian formulation of QFT. But in both formulations only under very special circumstances one can solve the ensuing equations, as for noninteracting theories or within some kind of mean field approximation.

In this MSc thesis we focus on the Wigner functional formalism of Ref. [11]. In the original publication, the authors employed a scalar field theory with quartic self-interactions. This formulation was extended to the electromagnetic field in Ref. [13] and to the Dirac field in Ref. [25]. In the original publication [11], the authors computed the finite temperature Wigner functional for the noninteracting free theory and also in the mean field approximation. In this thesis we transcribe to this QFT Wigner functional formalism a variational method developed in statistical mechanics to extend the traditional mean field approximation for the free energy of nonrelativistic many-body theories. This method was proposed in 1957 by Bogoliubov, Zubarev and Tserkovnikov [26]. These authors made the crucial observation that the Gibbs variational method applied to the free energy of a reduced BCS Hamiltonian[1] yields the exact grand canonical potential of the model in the thermodynamical limit. The method was further developed by Wentzel [28] to the theory of superfluidity, who also coined the name "method of thermodynamically equivalent Hamiltonian". Later on, the method was generalized by Girardeau [29] to a broader spectrum of applications. Since the variational method builds on the thermal density matrix, one can use the method together with the formalism of Ref. [11] to obtain a Wigner functional that goes beyond the mean field approximation. To our knowledge, the use of such a variational method together with the phase space quantization is a novel formalism to treat nonperturbative problems in quantum field theory.

The key idea of the method is to identify a number of scattering processes in the Hamiltonian of the model such that one obtains a tractable problem by

[1] BCS stands for Bardeen, Cooper and Shriefer, who developed the first microscopic theory for the phenomenon of superconductivity in metals [27].

using a combination of the variational method and perturbation theory. The full Hamiltonian is split into two parts, one is quadratic in the fields and the other is nonquadratic. The quadratic part contains only those selected processes and can be diagonalized through a linear unitary transformation that depends on trial gap functions determined by the Gibbs variational principle. The nonquadratic part, that also depends on the trial functions, should be treated by perturbation theory. The chosen scattering processes should capture most of the physics of the problem. The method, however, does not provide a criterion for choosing one or another process, the choice should be guided by the problem of interest. The traditional mean field approximation, in particular, refers to the direct and exchange scattering processes in the Hamiltonian. In this study we abstract from any specific problem, and treat the method in its full generality.

We follow closely Ref. [11] for the Wigner functional formalism and Ref. [29] for the variational method. As in Ref. [11], we use a scalar field theory with quartic selfinteractions in $1+1$ dimensions. The model is well suited for our purposes since we can easily contrast the mean field formulation in Ref. [11] with the variational approach. But the simplicity of the model comes with a price, it is not rich enough for phenomenologically interesting applications. Besides the inherent limitations of one-dimensional scattering, a real scalar field theory cannot describe phenomena like superfluidity, condensate formation and phase transition phenomena. As such, it also limits our capability to assess numerically the impact of the variational method on observables. In any case, such limitations are not of fundamental importance; the model reveals general features of the method that will be present in a phenomenologically more realistic model.

We divide the thesis into five chapters and four appendices. In Chapter 2 we make a concise revision of quantum field theory topics which will be useful throughout the text, namely the path integral formalism and generating functionals. In Chapter 3, we review Wigner's phase space quantization formalism. We start with the formalism in quantum mechanics, which will be very brief and far from exhaustive. Then we review the QFT phase space formalism of Ref. [11]. Chapter 4 contains our original contribution to the Wigner functional theory in quantum field theory (QFT). We discuss the formalism of the variational method of Ref. [29], and in some parts we use material from the thesis work in Ref. [30]. We show how the traditional mean field approximation for the Wigner functional arises within the variational method. We also present results from a numerical exercise to explore features of the formalism. We solved numerically the gap

equation and obtained the eigenvalues and eigenfunctions of the quadratic Hamiltonian. We use those results to compute a two-point correlation function and the 2^{nd}-Rényi entropy. Chapter 5 presents a conclusion and discusses perspectives for future work. The four appendices supplement with mathematical proofs many of the results used in the body of the work.

Chapter 2

Path Integral Formalism

The quantum field theory (QFT) Wigner functional formalism we consider in this dissertation uses path integrals. Explicit computations require techniques similar to those used in the traditional QFT path integral quantization. In this chapter we present a brief review of the path integral quantization formalism with the sole aim of presenting the main computation techniques that we use in the following chapters. We start reviewing the formalism for quantum mechanics and then generalize it to QFT.

The basis of the path quantization procedure is wave mechanics, similar in form to the Huygens-Fresnel principle. The mathematical framework of path integral was known by mathematicians from the work of Wiener in the study of stochastic processes. A few references to the work of mathematicians on this subject can be found in the review paper by Gelfand and Yaglom [31].

The original idea on path integrals in physics, as pointed in the introduction of Feynman's paper [32], is due to "Dirac's remarks concerning the relation of classical action to quantum mechanics" [33, 34, 35]. We can read in those Dirac's works his search for a close relation between the classical and quantum mechanics, even more in the section "The Action Principle" in his quantum mechanics book [34]. In 1949, Dyson [36] proposed "a unified development of the subject of quantum electrodynamics", grounding the path integral formalism as a fully equivalent method of quantization to those developed at the time in quantum electrodynamics. We follow in this chapter the presentation in the textbook of Schwartz [37]. The interested reader can also find useful texts in the classical book Peskin and Schröder [38], or Zee [39] for beginners. We will also make use of Pokorski's book [40] for some topics. As mentioned in the introduction, shall use $\hbar = c = 1$ throughout this chapter.

2.1 Path Integral in Quantum Mechanics

In non-relativistic quantum mechanics the most general Hamiltonian in one-dimension is of the form:

$$\hat{H}(t) = \frac{\hat{p}^2}{2m} + \hat{V}(\hat{x}, t)\,, \tag{2.1}$$

where $V(\hat{x}, t)$ is the potential; t is the time (not an operator). When $\hat{V}$ is t-independent, the probability amplitude for a transition from a state $|\, i \,\rangle = |\, x_i, t_i \,\rangle$ to a state $|\, f \,\rangle = |\, x_f, t_f \,\rangle$ in the Heisenberg representation is given by:

$$\langle f|i\rangle = \langle x_f, t_f | x_i, t_i\rangle = \langle x_f | e^{-i(t_f - t_i)\hat{H}} | x_i\rangle\,. \tag{2.2}$$

When $\hat{V}$ is time-dependent, one can use such a formula only if the time interval $t_f - t_i$ is sufficiently small; when the time interval is not small, and $\hat{V}$ is a smooth function of t, we can evolve the amplitude by splitting the time interval into small δt steps and take $\delta t \to 0$ at the end of the calculation. This proceeds as follows: we define $t_j = t_i + j\,\delta t$, with $t_n = t_f$, and write

$$\langle f|i\rangle = \int dx_n ... dx_1 \langle x_f | e^{-iH(t_n)\delta t} | x_n\rangle \langle x_n | \cdots | x_2\rangle \langle x_2 | e^{-iH(t_1)\delta t} | x_1\rangle \langle x_1 | e^{-iH(t_i)\delta t} | x_i\rangle, \tag{2.3}$$

where we inserted n complete sets of position eigenstates through the completeness relationship $\int dx_j\, |x_j\rangle\langle x_j| = \mathbb{1}$, and defined $\hat{H}(t_j) = \hat{p}^2/2m + \hat{V}(\hat{x}, t_j)$. To evaluate each matrix element, we insert a complete set of momentum eigenstates through $\mathbb{1} = \int dp\, |p\rangle\langle p|$ and use the (unnormalized) plane wave $\langle x|p\rangle = e^{ipx}$, so that:

$$\begin{aligned} \langle x_{j+1} | e^{-iH\delta t} | x_j\rangle &= \int dp \langle x_{j+1} |\, p\,\rangle \langle\, p\, | e^{-i[\frac{\hat{p}^2}{2m} + V(\hat{x}_j, t_j)]\,\delta t} |\, x_j\,\rangle \\ &= e^{-iV(\hat{x}_j, t_j)\delta t} \int dp\, e^{-i\frac{\hat{p}^2}{2m}\delta t} e^{i\,p\,(x_{j+1} - x_j)}\,. \end{aligned} \tag{2.4}$$

Now, we can use Eq. (A.10) from Appendix A to compute the momentum integral:

$$\langle x_{j+1} | e^{-iH\delta t} | x_j\rangle = N\, e^{-iV(\hat{x}_j, t_j)\delta t} e^{i\frac{m}{2}\frac{(x_{j+1} - x_j)^2}{(\delta t)^2}\delta t} = N\, e^{i\left(\frac{m}{2}\frac{(x_{j+1} - x_j)^2}{(\delta t)^2} - V(x_j, t_j)\right)\delta t}, \tag{2.5}$$

where N is a constant (independent of x and t) which, as we argue shortly ahead, plays no role in the final result. We are then able to write the matrix element as

$$\langle x_{j+1}|e^{-iH\delta t}|x_j\rangle \;=\; N\, e^{i\left(\frac{m}{2}\frac{(x_{j+1}-x_j)^2}{(\delta t)^2}-V(x_j,t_j)\right)\delta t} = N\, e^{iL(x,\dot{x})\,\delta t}, \tag{2.6}$$

where we anticipated that

$$\frac{(x_{j+1}-x_j)^2}{(\delta t)^2} \xrightarrow[\delta t\to 0]{} \dot{x}^2\,, \tag{2.7}$$

with

$$L(x,\dot{x}) = \frac{1}{2}m\dot{x}^2 - V(x,t)\,, \tag{2.8}$$

being the Lagrangian. We see that this procedure implemented a Legendre transform from the Hamiltonian $H(x,p)$ to the Lagrangian $L(x,\dot{x})$. The whole probability amplitude can now be written as

$$\begin{aligned}\langle f|i\rangle \;&=\; N^n \int_{x(t_i)=x_i}^{x(t_f)=x_f} dx_n\, e^{iL(x_n,\dot{x}_n)dt}\,\cdots dx_1\, e^{iL(x_1,\dot{x}_1)dt}\\ &=\; \prod_n N \int_{x(t_i)=x_i}^{x(t_f)=x_f} dx_n\, e^{iL(x_n,\dot{x}_n)dt} \xrightarrow[\delta t\to 0]{} \int Dx_n\; e^{iS[x]}\,,\end{aligned} \tag{2.9}$$

where

$$S[x] = \int dt\, L(x,\dot{x})\,, \tag{2.10}$$

is the action, and

$$\int Dx_n = \prod_{n=1}^{\infty} N \int_{x(t_i)=x_i}^{x(t_f)=x_f} dx_n\,, \tag{2.11}$$

is the functional measure. N is a formally infinite constant that drops out when one computes any physical quantity because physical quantities involve ratios of path integrals with this measure. In the next section we will see this more explicitly. The moral of the story is that the transition probability amplitude between an initial and a final position state is given by an infinite sum over classical trajectories, including the ones that do not satisfy the classical equations of motion (i.e. not derived from the minimal action principle).

We note that this procedure, albeit giving equivalent results to the ordinary Hilbert space operator formalism, has its advantages and disadvantages. It would be cumbersome to solve the hydrogen atom, for example, with this method,

but it proves extremely useful in many-particle systems and relativistic QFT. Reference [41] presents a collection of solved nonrelativistic quantum mechanics problems using the path integral approach. We also refer the interested reader to the classical quantum mechanics textbook of Sakurai and Napolitano [42].

2.1.1 Generating Functional

As a further step toward introducing the path integral formalism in QFT, we consider the matrix element of the product of position operators $\hat{x}(t)$ "sanduiched" between two position eigenstates. These position operators will be replaced by field operators $\hat{\Phi}(x)$ in the QFT formalism in Section 2.2.

Let us consider first such a matrix element for two position operators, namely $\langle x', t'|\hat{x}(t_1)\hat{x}(t_2)|x, t\rangle$, with t_1 and t_2 within the $t' - t$ time interval. We proceed as above: we divide the time interval $t' - t$ into small time steps and insert complete sets of position and momentum eigenstates through the corresponding completeness relationships. To avoid clutter due to proliferation of indices, we change $t_1 \to \tau_1$ and $t_2 \to \tau_2$ and reinstate t_1 and t_2 at the end. Specifically, we choose the intermediate times $t_n > \cdots > t_1$ such that for $\tau_1 > \tau_2$ with τ_1 being the i_1-th time step and τ_2 the i_2-th step,

$$\tau_1 = t_{i_1}, \qquad \tau_2 = t_{i_2}\,, \tag{2.12}$$

so that we can write

$$\begin{aligned}
\langle x', t'|\hat{x}(\tau_1)\hat{x}(\tau_2)|x, t\rangle &= \int dx_n \ldots dx_{i_1} dx_{i_1-1} \ldots dx_{i_2} dx_{i_2-1} \ldots dx_1 \; \langle x', t'|x_n, t_n\rangle \\
&\quad \times \cdots \langle x_{i_1}, t_{i_1}|\hat{x}(\tau_1)|x_{i_1-1}, t_{i_1-1}\rangle \cdots \langle x_{i_2}, t_{i_2}|\hat{x}(\tau_2)|x_{i_2-1}, t_{i_2-1}\rangle \cdots \langle x_1, t_1|x, t\rangle \\
&= \int dx_n \ldots dx_{i_1} dx_{i_1-1} \ldots dx_{i_2} dx_{i_2-1} \ldots dx_1 \; x_{i_1}\, x_{i_2} \, \langle x', t'|x_n, t_n\rangle \\
&\quad \times \cdots \langle x_{i_1}, t_{i_1}|x_{i_1-1}, t_{i_1-1}\rangle \cdots \langle x_{i_2}, t_{i_2}|x_{i_2-1}, t_{i_2-1}\rangle \cdots \langle x_1, t_1|x, t\rangle\,.
\end{aligned} \tag{2.13}$$

Each of the scalar products in this expression is given by the result in Eq. (2.6), so

that:

$$\begin{aligned}\langle x', t'|\hat{x}(\tau_1)\hat{x}(\tau_2)|x, t\rangle &= N^n \int dx_n \dots dx_{i_1} dx_{i_1-1} \dots dx_{i_2} dx_{i_2-1} \dots dx_1 \\ &\times\ x_{i_1}\, x_{i_2}\, e^{iL(x_n,\dot{x}_n)\,\delta t} \dots\ e^{iL(x_{i_1},\dot{x}_{i_1})\,\delta t}\ \dots\ e^{iL(x_{i_2},\dot{x}_{i_2})\,\delta t}\ \dots\ e^{iL(x_1,\dot{x}_1)\,\delta t} \\ &\xrightarrow[\delta t\to 0]{} \int Dx_n\ x(\tau_1)\, x(\tau_2)\ e^{iS[x]}\,. \end{aligned} \tag{2.14}$$

The above manipulations are valid only for $\tau_1 > \tau_2$, because of the choice indicated in Eq. (2.12); if $\tau_1 < \tau_2$ the result in Eq. (2.14) would correspond to the matrix element $\langle x', t'|\hat{x}(\tau_2)\hat{x}(\tau_1)|x, t\rangle$, as one can check by repeating the calculation for this case. So path integrals like Eq. (2.14) define the matrix elements of time-ordered products of position operators:

$$\int Dx\, x(t_1)x(t_2)\, e^{iS[x]} = \begin{cases} \langle x', t'|\hat{x}(t_1)\hat{x}(t_2)|x, t\rangle & \text{for } t_1 > t_2\,, \\ \langle x', t'|\hat{x}(t_2)\hat{x}(t_1)|x, t\rangle & \text{for } t_1 < t_2, \end{cases} \tag{2.15}$$

$$= \langle x', t'|T\hat{x}(t_1)\hat{x}(t_2)|x, t\rangle\,. \tag{2.16}$$

This result generalizes to matrix elements of time-order products of several position operators [40]:

$$\langle x', t'|\hat{x}(t_1)\cdots\hat{x}(t_n)|x, t\rangle = \int Dx\, x(t_1)\cdots x(t_n)\, e^{iS[x]}\,. \tag{2.17}$$

One can obtain the transition amplitude in the presence of a classical external source $J(\tau)$ as

$$\langle x', t'|x, t\rangle_J = \int Dx\ e^{i\int_t^{t'} d\tau\,\left[L(x,\dot{x})+J(\tau)x(\tau)\right]}\,, \tag{2.18}$$

by modifying the Hamiltonian by a source term: $H \longrightarrow H - Jx$. This path integral can be used as generating functional of the matrix elements of position operators, which can be evaluated through

$$\langle x', t'|T\hat{x}(t_1)\cdots\hat{x}(t_n)|x, t\rangle = \left(\frac{1}{i}\right)^n \frac{\delta^n}{\delta J(t_1)\dots\delta J(t_n)} \langle x', t'|x, t\rangle_J \Big|_{J=0}\,. \tag{2.19}$$

Here, the functional derivative with respect to J of a given functional $F[J]$

$$F[J] = \int dx_1 ... \int dx_n \, f(x_1 ... x_n) J(x_1) ... J(x_n) \,, \tag{2.20}$$

is given by

$$\frac{\delta F[J]}{\delta J(x)} = \int dx_1 ... \int dx_{n-1} \, n \, f(x_1 ... x_{n-1}, x) J(x_1) ... J(x_{n-1}) \,, \tag{2.21}$$

which corresponds to the usual rule of differentiating monomials.

2.1.2 Vacuum to Vacuum Transition

In QFT we are often interested in matrix elements of products of field operators in the vacuum state, i.e. in the ground state of the Hamiltonian. Those matrix elements relate to Green's functions which contain spectral information on single and many-particle states. Such a matrix element can also be obtained through a generating functional, as we show next by following Ref. [40].

We consider a time-independent Hamiltonian. We denote by $|n\rangle$ its energy eigenstates, with $|0\rangle$ being the ground state (the vaccum state); the corresponding coordinate-space representation are $\psi_n(x) = \langle x|n\rangle$ and $\psi_0(x) = \langle x|0\rangle$. The matrix element $\langle 0|T\left[\hat{x}(t_1)\cdots\hat{x}(t_n)\right]|0\rangle$ can be written as

$$\begin{aligned}\langle 0|T\left[\hat{x}(t_1)\cdots\hat{x}(t_n)\right]|0\rangle &= \int dx' dx \, \langle 0|x',t'\rangle \, \langle x',t'|T\hat{x}(t_1)\cdots\hat{x}(t_n)|x,t\rangle \, \langle x,t|0\rangle \\ &= \int dx' dx \, \psi_0^*(x',t') \, \langle x',t'|T\hat{x}(t_1)\cdots\hat{x}(t_n)|x,t\rangle \, \psi_0(x,t). \end{aligned} \tag{2.22}$$

The aim is to obtain a generating functional $Z[J]$ from which one can obtain this vacuum-to-vacuum matrix element as

$$\left(\frac{1}{i}\right)^n \frac{\delta^n}{\delta J(t_1)...\delta J(t_n)} Z[J] \,\Bigg|_{J=0} . \tag{2.23}$$

That such a generating functional exists is clear from Eq. (2.19) as one can use it in Eq. (2.22) for $\langle x',t'|T\left[\hat{x}(t_1)\cdots\hat{x}(t_n)\right]|x,t\rangle$. But this does not give a very convenient expression because it needs $\psi_0(x,t)$. Let us show how to obtain a more practical expression for the generating functional.

As a first step, we consider the transition amplitude $\langle x_2, T_2|x_1, T_1\rangle$, where T_1

and T_2 are arbitrary time instants. We rewrite this amplitude as

$$\langle x_2, T_2|x_1, T_1\rangle = \int dx dx' \, \langle x_2, T_2|x', t'\rangle \, \langle x', t'|x, t\rangle \, \langle x, t|x_1, T_1\rangle. \tag{2.24}$$

Next, we assume a source $J(t)$ vanishing at all times except for those in the interval (t, t'), with $T_2 > t' > t > T_1$; therefore, one can write

$$\langle x_2, T_2|x_1, T_1\rangle_J = \int dx' dx \, \langle x_2, T_2|x', t'\rangle \, \langle x', t'|x, t\rangle_J \, \langle x, t|x_1, T_1\rangle \, . \tag{2.25}$$

The time dependence of the source-free amplitudes $\langle x_2, T_2|x', t'\rangle$ and $\langle x, t|x_1, T_1\rangle$ is made explicit by using the eigenstates of the source-free Hamiltonian as follows:

$$\langle x, t|x_1, T_1\rangle = \langle x|e^{-i\hat{H}(t-T_1)}|x_1\rangle = \sum_n \psi_n(x) \, \psi_n^*(x_1) \, e^{-iE_n(t-T_1)} \, , \tag{2.26}$$

$$\langle x_2, T_2|x', t'\rangle = \langle x_2|e^{-i\hat{H}(T_2-t')}|x'\rangle = \sum_n \psi_n(x_2) \, \psi_n^*(x') \, e^{-iE_n(T_2-t')} \, . \tag{2.27}$$

To pick up the ground state we are interested in, we multiply the matrix element in Eq. (2.26) by $e^{-iE_0T_1}$ and continue $T_1 \to +i\infty$. In this limit, the largest contribution comes from the lowest energy eigenvalue E_0 and so:

$$\lim_{T_1 \to +i\infty} \left[e^{-iE_0T_1} \langle x, t|x_1, T_1\rangle \right] = \psi_0(x) \, e^{-iE_0t} \, \psi_0^*(x_1) = \psi_0(x, t) \, \psi_0^*(x_1) \, . \tag{2.28}$$

The same is true for the matrix element in Eq. (2.27) with $T_2 \to -i\infty$:

$$\lim_{T_2 \to -i\infty} \left[e^{iE_0T_2} \langle x_2, T_2|x', t'\rangle \right] = \psi_0^*(x', t') \, \psi_0(x_2) \, . \tag{2.29}$$

We can now use these results in Eq. (2.25) to obtain:

$$\lim_{\substack{T_1 \to +i\infty \\ T_2 \to -i\infty}} \frac{\langle x_2, T_2|x_1, T_1\rangle_J}{e^{-iE_0(T_2-T_1)} \psi_0^*(x_2) \psi_0(x_1)} = \int dx dx' \, \psi_0^*(x', t') \, \langle x', t'|x, t\rangle_J \, \psi_0(x, t) \, . \tag{2.30}$$

Therefore, up to J-independent factors, $Z[J]$ is given by the left hand side of this expression. We note that the J-independent factors drop out when normalizing $\langle 0|T\left[\hat{x}(t_1) \cdots \hat{x}(t_n)\right]|0\rangle$ by the vacuum-to-vacuum transition amplitude $\langle 0|0\rangle$. Specifically, first we note that the right hand side of Eq. (2.30) for $J = 0$ is nothing

else than $\langle 0|0\rangle$, which, by Eq. (2.18) with $J = 0$, is given by

$$\langle 0|0\rangle = \lim_{\substack{T_1\to+i\infty \\ T_2\to-i\infty}} \frac{\int Dx\, e^{i\int_{T_1}^{T_2} dt\, L(x,\dot{x})}}{e^{-iE_0(T_2-T_1)}\psi_0^*(x_2)\psi_0(x_1)}\,. \tag{2.31}$$

Then, we use Eqs. (2.18) and (2.19) with Eq. (2.30) to obtain

$$\begin{aligned}\langle 0|T\hat{x}(t_1)\cdots\hat{x}(t_n)|0\rangle &= \frac{\langle 0|T\left[\hat{x}(t_1)\cdots\hat{x}(t_n)\right]|0\rangle}{\langle 0|0\rangle} \lim_{\substack{T_1\to+i\infty \\ T_2\to-i\infty}} \frac{\int Dx\, e^{i\int_{T_1}^{T_2} dt\, L(x,\dot{x})}}{e^{-iE_0(T_2-T_1)}\psi_0^*(x_2)\psi_0(x_1)} \\ &= \left(\frac{1}{i}\right)^n \frac{\delta^n}{\delta J(t_1)...\delta J(t_n)} \lim_{\substack{T_1\to+i\infty \\ T_2\to-i\infty}} \frac{\int Dx\, e^{i\int_{T_1}^{T_2} dt\left[L(x,\dot{x})+J(t)x(t)\right]}}{e^{-iE_0(T_2-T_1)}\psi_0^*(x_2)\psi_0(x_1)}\Bigg|_{J=0}\end{aligned} \tag{2.32}$$

Cancelling the common factor $e^{-iE_0(T_2-T_1)}\psi_0^*(x_2)\psi_0(x_1)$, we can then write

$$\frac{\langle 0|T\left[\hat{x}(t_1)\cdots\hat{x}(t_n)\right]|0\rangle}{\langle 0|0\rangle} = \frac{1}{Z[0]}\left(\frac{1}{i}\right)^n \frac{\delta^n}{\delta J(t_1)...\delta J(t_n)} Z[J]\Bigg|_{J=0}\,, \tag{2.33}$$

with $Z[J]$ given by:

$$Z[J] = \lim_{\substack{T_1\to+i\infty \\ T_2\to-i\infty}} \int_{x(T_1)}^{x(T_2)} Dx\, e^{i\int_{T_1}^{T_2} dt\left[L(x,\dot{x})+J(t)x(t)\right]}\,, \tag{2.34}$$

where we made explicit in the path integral the arbitrary end-point trajectories $x(T_1)$ and $x(T_2)$.

2.2 Path Integral in Quantum Field Theory

In this section we transcribe the previous formalism to QFT. We exemplify the formalism for a real scalar field theory with self interaction $\frac{\lambda}{4!}\Phi^4$, which is the theory that we use to discuss the Wigner formulation. In QFT, it is usual to define the theory through a Lagrangian density and then obtain the corresponding Hamiltonian to define the path integral. The Lagrangian density is given by

$$\mathcal{L} = \frac{1}{2}\,\partial_\mu\Phi\partial^\mu\Phi - \frac{1}{2}m^2\Phi^2 - \frac{\lambda}{4!}\Phi^4 = \frac{1}{2}\left(\dot{\Phi}^2 - (\nabla\Phi)^2\right) - V(\Phi)\,, \tag{2.35}$$

with

$$V(\Phi) = \frac{1}{2}m^2\Phi^2 + \frac{\lambda}{4!}\Phi^4 \,. \tag{2.36}$$

The spacetime dependence of the field is $\Phi(x) = \Phi(\mathbf{x}, t)$ and, as usual, $\dot{\Phi} = \partial\Phi/\partial t$. The classical conjugate momentum $\Pi(x)$ is then

$$\Pi(x) = \frac{\partial \mathcal{L}}{\partial \dot{\Phi}(x)} \,. \tag{2.37}$$

By Legendre transforming this Lagrangian, one obtains the classical Hamiltonian density:

$$\mathcal{H} = \frac{1}{2}\Big(\Pi^2 + (\nabla\Phi)^2\Big) + V(\Phi) \,, \tag{2.38}$$

One can follow the same steps of the previous section to quantize the theory by identifying the position $\hat{\mathbf{x}}(t)$ and momentum $\hat{\mathbf{p}}(t)$ Heisenberg representation operators with the field operators $\hat{\Phi}(\mathbf{x}, t)$ and $\hat{\Pi}(\mathbf{x}, t)$, respectively. That is, there is one dynamical variable at each spacetime position $(\mathbf{x}, t)$. The corresponding equal-time commutation relations are (recall we are using $\hbar = 1$):

$$[\,\hat{\Phi}(\mathbf{x}, t), \hat{\Phi}(\mathbf{y}, t)\,] = [\,\hat{\Pi}(\mathbf{x}, t), \hat{\Pi}(\mathbf{y}, t)\,] = 0 \,, \tag{2.39}$$

$$[\,\hat{\Phi}(\mathbf{x}, t), \hat{\Pi}(\mathbf{y}, t)\,] = i\delta^d(\mathbf{x} - \mathbf{y}) \,, \tag{2.40}$$

where d is the spatial dimensionality; the spacetime diemensionality is $d + 1$. The field theory "coordinate" representation is formally characterized by

$$\hat{\Phi}(\mathbf{x})|\Phi\rangle = \Phi(\mathbf{x})|\Phi\rangle \,, \tag{2.41}$$

in that one thinks of a "lattice" representation of the state vectors $|\Phi(\mathbf{x})\rangle$ [43]:

$$|\Phi\rangle = \prod_{\mathbf{x}} |\Phi(\mathbf{x})\rangle \,, \tag{2.42}$$

$$\langle\Phi|\Phi'\rangle = \prod_{\mathbf{x}} \delta\big(\Phi(\mathbf{x}) - \Phi'(\mathbf{x})\big) \,, \tag{2.43}$$

$$\prod_{\mathbf{x}} \int_{-\infty}^{\infty} d\Phi(\mathbf{x})\, |\Phi(\mathbf{x})\rangle\langle\Phi(\mathbf{x})| = \mathbb{1} \,, \tag{2.44}$$

and similar expressions for the eigenstates $|\Pi\rangle$ of the $\hat{\Pi}(\mathbf{x})$ operator.

It will be useful for the developments throughout this dissertation to go over momentum space. We define the momentum space $\hat{\Phi}(\mathbf{p}, t)$ and $\hat{\Pi}(\mathbf{p}, t)$ field

operators through the Fourier transforms:

$$\hat{\Phi}(\mathbf{p},t) = \int d^d x\, e^{-i\mathbf{p}\cdot\mathbf{x}}\,\hat{\Phi}(\mathbf{x},t)\,, \tag{2.45}$$

$$\hat{\Pi}(\mathbf{p},t) = \int d^d x\, e^{-i\mathbf{p}\cdot\mathbf{x}}\,\hat{\Pi}(\mathbf{x},t)\,. \tag{2.46}$$

The commutation relations of Eq. (2.39) and Eq. (2.40) are then given by

$$\begin{aligned}[\,\hat{\Phi}(\mathbf{p},t),\hat{\Pi}^\dagger(\mathbf{q},t)\,] &= \int d^d x\, d^d y\, e^{-i\mathbf{p}\cdot\mathbf{x}+i\mathbf{q}\cdot\mathbf{y}}\,[\,\hat{\Phi}(\mathbf{x},t),\hat{\Pi}(\mathbf{y},t)\,] \\ &= \int d^d x\, d^d y\, e^{-i\mathbf{p}\cdot\mathbf{x}+i\mathbf{q}\cdot\mathbf{y}}\, i\,\delta(\mathbf{x}-\mathbf{y}) \\ &= i\int d^d x\, e^{-i(\,\mathbf{p}-\mathbf{q}\,)\cdot\mathbf{x}} = i\,(2\pi)^d\delta^d(\mathbf{p}-\mathbf{q})\,. \end{aligned} \tag{2.47}$$

On the same steps, one finds

$$[\,\hat{\Phi}(\mathbf{p},t),\hat{\Phi}(\mathbf{q},t)\,] = [\,\hat{\Pi}(\mathbf{p},t),\hat{\Pi}(\mathbf{q},t)\,] = 0\,. \tag{2.48}$$

For a real scalar field, we have that

$$\Phi^\dagger(\mathbf{p},t) = \left(\int d^d x\, e^{-i\mathbf{p}\cdot\mathbf{x}}\,\hat{\Phi}(\mathbf{x},t)\right)^\dagger = \int d^d x\, e^{+i\mathbf{p}\cdot\mathbf{x}}\,\hat{\Phi}(\mathbf{x},t) = \Phi(-\mathbf{p},t)\,. \tag{2.49}$$

Therefore, the commutator of $\hat{\Phi}(\mathbf{p},t)$ and $\hat{\Phi}^\dagger(\mathbf{q},t)$ also vanishes:

$$[\,\hat{\Phi}(\mathbf{p},t),\hat{\Phi}^\dagger(\mathbf{q},t)\,] = \int d^d x\, d^d y\, e^{-i\mathbf{p}\cdot\mathbf{x}+i\mathbf{q}\cdot\mathbf{y}}\,[\,\hat{\Phi}(\mathbf{x},t),\hat{\Phi}(\mathbf{y},t)\,] = 0\,. \tag{2.50}$$

As in coordinate space, the field theory "coordinate" representation in momentum space is formally characterized by

$$\hat{\Phi}(\mathbf{p})|\Phi\rangle = \Phi(\mathbf{p})|\Phi\rangle\,, \tag{2.51}$$

and again it is understood that

$$|\Phi\rangle = \prod_{\mathbf{p}} |\Phi(\mathbf{p})\rangle\,, \tag{2.52}$$

$$\langle\Phi|\Phi'\rangle = \prod_{\mathbf{p}} \delta(\Phi(\mathbf{p}) - \Phi'(\mathbf{p}))\,, \tag{2.53}$$

$$\prod_{\mathbf{p}} \int_{-\infty}^{\infty} d\Phi(\mathbf{p})\, |\Phi(\mathbf{p})\rangle\langle\Phi(\mathbf{p})| = \mathbb{1}\,. \tag{2.54}$$

Finally, the coordinate representation of $|\Pi\rangle$ is given (up to a normalization constant) by

$$\langle\Phi|\Pi\rangle = e^{i\int d^d x\, \Pi(\mathbf{x})\Phi(\mathbf{x})}\,. \tag{2.55}$$

In an explicit lattice discretization, this is given by

$$\langle\Phi|\Pi\rangle = e^{ia^d \sum_x \Pi(\mathbf{x})\Phi(\mathbf{x})} = \prod_{\mathbf{x}} e^{ia^d\, \Pi(\mathbf{x})\Phi(\mathbf{x})} = \prod_x \langle\Phi(\mathbf{x})|\Pi(\mathbf{x})\rangle\,, \tag{2.56}$$

where a is the lattice spacing. One can express these relations in momentum space by Forier transforming the fields.

Next, we consider the QFT transition probability amplitude that generalizes $\langle x_f, t_f | x_i, t_i\rangle$:

$$\langle f|i\rangle = \langle\Phi_f|e^{-i(t_f - t_i)\hat{H}}|\Phi_i\rangle\,, \tag{2.57}$$

where Φ_i and Φ_f are the eigenstates of $\hat{\Phi}$ at the times t_i and t_f respectively. We proceed as in the quantum mechanical case by dividing $t_f - t_i$ into small δt pieces. But now we need the spatially discretized Hamiltonian as well, because we will use the discretized completeness relations of Eqs. (2.44) and (2.54). At this point, it suffices to replace the spatial integral over the Hamiltonian density by a discrete sum without entering into particular discretizations of spatial derivatives; specifically, it is sufficient to write the discretized Hamiltonian as:

$$\hat{H} = \int d^d x\, \mathcal{H} \to a^d \sum_{\mathbf{x}} \hat{\mathcal{H}}(\mathbf{x})\,, \tag{2.58}$$

with

$$\hat{\mathcal{H}}(\mathbf{x}) = \frac{1}{2}\Pi^2(\mathbf{x}) + \frac{1}{2}\left(\nabla\Phi(\mathbf{x})\right)^2 + V(\Phi(\mathbf{x}))\,. \tag{2.59}$$

We can proceed in a manner similar to that we proceeded in the previous section,

namely:

$$\begin{aligned}
\langle f|i\rangle &= \langle \Phi_f(\mathbf{x})|e^{-i(t_f-t_i)a^d\sum_{\mathbf{x}}\hat{\mathcal{H}}(\mathbf{x})}|\Phi_i(\mathbf{x})\rangle \\
&= \langle \Phi_f(\mathbf{x})|e^{-i\delta t\, a^d\sum_{\mathbf{x}}\hat{\mathcal{H}}(\mathbf{x})}\ \ldots\ e^{-i\delta t\, a^d\sum_{\mathbf{x}}\hat{\mathcal{H}}(\mathbf{x})}|\Phi_i(\mathbf{x})\rangle \\
&= \prod_{j_n}\int_{-\infty}^{\infty} d\Phi_{j_n}(\mathbf{x})\ \ldots \prod_{j_2}\int_{-\infty}^{\infty} d\Phi_{j_2}(\mathbf{x})\ \prod_{j_1}\int_{-\infty}^{\infty} d\Phi_{j_1}(\mathbf{x}) \\
&\quad \times \langle \Phi_f(\mathbf{x})|e^{-i\delta t\, a^d\hat{\mathcal{H}}_{j_n}(\mathbf{x})}|\Phi_{j_n}(\mathbf{x})\rangle\ \cdots\ \langle \Phi_{j_2}(\mathbf{x})|e^{-i\delta t\, a^d\hat{\mathcal{H}}_{j_1}(\mathbf{x})}|\Phi_{j_1}(\mathbf{x})\rangle \\
&\quad \times \langle \Phi_{j_1}(\mathbf{x})|e^{-i\delta t\, a^d\hat{\mathcal{H}}_{i}(\mathbf{x})}|\Phi_{i}(\mathbf{x})\rangle\,. \qquad (2.60)
\end{aligned}$$

Each matrix element is evaluated by inserting the momentum completeness relation given by Eq. (2.54); for a generic $(j+1, j)$ matrix element, we obtain:

$$\begin{aligned}
\langle \Phi_{j+1}(\mathbf{x})|e^{-i\delta t\, a^d\hat{\mathcal{H}}_{j}(\mathbf{x})}|\Phi_{j}(\mathbf{x})\rangle &= e^{-i\delta t\, a^d\left[\frac{1}{2}\left(\nabla\Phi_j(\mathbf{x})\right)^2+V(\Phi_j(\mathbf{x}))\right]} \\
&\quad \times \prod_{k}\int_{-\infty}^{\infty} d\Pi_k(\mathbf{x})\, e^{-i\delta t\, a^d\,\frac{1}{2}\,\Pi_k^2(\mathbf{x})}\,\langle \Phi_{j+1}(\mathbf{x})|\Pi_k(\mathbf{x})\rangle\,\langle \Pi_k(\mathbf{x})|\Phi_j(\mathbf{x})\rangle \\
&= e^{-i\delta t\, a^d\left[\frac{1}{2}\left(\nabla\Phi_j(\mathbf{x})\right)^2+V(\Phi_j(\mathbf{x}))\right]} \\
&\quad \times \int_{-\infty}^{\infty} d\Pi_j(\mathbf{x})\, e^{-i\delta t\, a^d\,\frac{1}{2}\,\Pi_j^2(\mathbf{x})}\, e^{i\delta t\, a^d\left(\frac{\Phi_{j+1}(\mathbf{x})-\Phi_j(\mathbf{x})}{\delta t}\right)\Pi_j(\mathbf{x})} \\
&= N\, e^{-i\delta t\, a^d\left[-\frac{1}{2}\left(\frac{\Phi_{j+1}(\mathbf{x})-\Phi_j(\mathbf{x})}{\delta t}\right)^2+\frac{1}{2}\left(\nabla\Phi_j(\mathbf{x})\right)^2+V(\Phi_j(\mathbf{x}))\right]} \\
&= N\, e^{i\delta t\, a^d\left[\frac{1}{2}\dot{\Phi}_j^2(\mathbf{x})-\frac{1}{2}\left(\nabla\Phi_j(\mathbf{x})\right)^2-V(\Phi_j(\mathbf{x}))\right]} = N\ e^{i\delta t\, a^d\,\mathcal{L}(\Phi,\dot{\Phi})}, \qquad (2.61)
\end{aligned}$$

where we used Eq. (2.56) for the lattice plane wave, and Eq. (2.35) to identify the Lagrangian density. Then, we can write the probability amplitude as the path integral:

$$\langle f|i\rangle = \langle \Phi_f|e^{-i(t_f-t_i)\hat{H}}|\Phi_i\rangle = \int D\Phi(\mathbf{x},t)\, e^{iS[\Phi]}\,, \qquad (2.62)$$

where the action is given by

$$S[\Phi] = \int_{t_i}^{t_f} dt \int d^d x\, \mathcal{L}(\Phi,\dot{\Phi})\,, \qquad (2.63)$$

and the path integral is over all field functions $\Phi(\mathbf{x},t)$ with the boundary condi-

tions $\Phi(\mathbf{x}, t_i) = \Phi_i(\mathbf{x})$ and $\Phi(\mathbf{x}, t_f) = \Phi_f(\mathbf{x})$.

The generating functional in QFT can be derived in close analogy with what was done for quantum mechanics in the previous section. As said there, this provides a convenient way to calculate correlation functions using classical sources in a formalism similar to partition functions in statistical mechanics [44]. The generating functional in configuration space for a source $J(x)$ in field theory can be written as

$$Z[J] = \int D\Phi \, \exp\left[iS[\Phi] + i\int d^d x \, J(x)\Phi(x)\right] . \tag{2.64}$$

To evaluate a one-point correlation function, i.e. the vacuum expectation value of the field $\hat{\Phi}$, one needs to take a single functional derivative of $Z[J]$:

$$\begin{aligned} \frac{1}{Z[0]}\left(\frac{1}{i}\right)\frac{\partial Z}{\partial J(x_1)}\Big|_{J=0} &= \int D\Phi \, \Phi(x_1) \, \exp\left[iS[\Phi] + i\int d^d x J(x)\Phi(x)\right]_{J=0} \\ &= \langle 0|\hat{\Phi}(x_1)|0\rangle \, , \end{aligned} \tag{2.65}$$

in which the vacuum state is supposed to be normalized so that one can omit the $\langle 0|0\rangle$ normalization. For n-point correlation functions this generalizes to

$$\langle 0|T\hat{\Phi}(x_1)...\hat{\Phi}(x_n)|0\rangle = \frac{1}{Z[0]}\left(\frac{1}{i}\right)^n \frac{\delta^n Z[J]}{\delta J(x_1)...\delta J(x_n)}\Bigg|_{J=0} . \tag{2.66}$$

To conclude, let us reiterate that we will not use the path integral quantization formalism as outlined in this chapter. As said previously, we discussed it mainly because we need the calculation techniques reviewed above, familiar from most modern QFT textbooks, to discuss the Wigner functional quantization formalism, that is our focus in this dissertation.

Chapter 3

Wigner Functional Formalism

3.1 Quantum Mechanics in Phase Space

We can formulate quantum mechanics in phase space in analogy with classical mechanics. This procedure, also termed "Moyal quantization" or deformation quantization is grounded in the seminal work of Wigner quasi-distribution function [2] and on the Weyl's mapping of c-numbers into Hilbert space operators [45]; Dirac in 1930 [46] was the first to propose a formulation of quantum mechanics in phase space though, describing a function in this space obtained by a Fourier transform on the density matrix, but without success. Many attempts were made to further generalize this quantum mechanics, like the works of Moyal [47] and Groenewold [48] on the so called "star product" (or Moyal-Groenewold product) and the Sympletic Quantum Mechanics due to Viana et al [49].

Phase space dynamics is very useful in classical mechanics and it comes naturally from the Hamiltonian formulation. The attempts to extend this concept to embrace quantum mechanics were the drivers of many works, in the pursue of a general framework where classical mechanics can be smoothly recovered from phase space quantum mechanics as the Planck constant $\hbar$ goes to 0, i.e. this constant parametrizes the link between mechanics. An advantage of it is that under this formalism we can perform canonical transformations just like classical Hamiltonian mechanics [50]

Wigner's main objective was to introduce quantum corrections for statistical mechanics in the framework of phase space, but along the time his work evolve to a brand new version of quantum mechanics [3, 4] reproducing the nonrelativistic Schrodinger equation [49] along with many old results like the hydrogen atom solution [51, 52], and the Klein-Gordon [14] and Dirac [16] relativistic equations. In this chapter we shall follow mainly Viana et al [4] and Ballentine textbook [53]. We restore $\hbar$ because it will be important now on.

3.1.1 Definition and Properties

In this formalism, every operator $\hat{A}$ in Hilbert space $\mathcal{H}$ is associated to some complex function $A_w(x,p)$ in the phase space Γ. This procedure consist of a mapping so that the associative algebra of operators in $\mathcal{H}$ corresponds to an associative (but non-commutative) algebra in Γ. The interpretation of phase space quantum mechanics lies in the so called "Wigner function" $f_w(x,p)$ [2], defined as the Fourier transform of the density matrix, where both the position x and momentum p are c-numbers (in contrast to canonical quantum mechanics where they are operators in some Hilbert space $\mathcal{H}$). We define this function as

$$f_w(x,p) = (2\pi\hbar)^{-1} \int_{-\infty}^{\infty} dy \, \langle x - \frac{y}{2} | \, \hat{\rho} \, | x + \frac{y}{2} \rangle \, e^{\frac{ipy}{\hbar}} \, . \tag{3.1}$$

Similarly, we can define

$$f_w(x,p) = (2\pi\hbar)^{-1} \int_{-\infty}^{\infty} dk \, \langle p - \frac{k}{2} | \, \hat{\rho} \, | p + \frac{k}{2} \rangle \, e^{\frac{ikx}{\hbar}} \, . \tag{3.2}$$

The generalization to three dimensions and N particles is straightforward

$$f_w(\mathbf{r},\mathbf{p}) = (2\pi\hbar)^{-3N} \int_{-\infty}^{\infty} d^{3N}R \, \langle \mathbf{r} - \frac{\mathbf{R}}{2} | \, \hat{\rho} \, | \mathbf{r} + \frac{\mathbf{R}}{2} \rangle \, e^{\frac{i\mathbf{p}\cdot\mathbf{R}}{\hbar}} \, , \tag{3.3}$$

where $\mathbf{r}$ and $\mathbf{R}$ are three dimensional entities. We can show that Wigner function yields the probability density in configuration space through

$$\int dp \, f_w = |\psi(x)|^2 = \langle x | \, \hat{\rho} \, | x \rangle \, , \tag{3.4}$$

which allows us to find the probability density of find some particle between x and $x + dx$. We can prove this using the definition in Eq. (3.1) in one dimension, without loss of generality:

$$\begin{aligned} \int dp \, f_w(x,p) &= (2\pi\hbar)^{-1} \int dy dp \, \langle x - \frac{y}{2} | \, \hat{\rho} \, | x + \frac{y}{2} \rangle \, e^{\frac{ipy}{\hbar}} \\ &= \int dy \, \langle x - \frac{y}{2} | \, \rho \, | x + \frac{y}{2} \rangle \left[(2\pi\hbar)^{-1} \int dp \, e^{\frac{ipy}{\hbar}} \right] . \end{aligned} \tag{3.5}$$

The integral between square brackets is a Dirac delta $\delta(y)$, so we write

$$\int dp \, f_w(x,p) = \langle x | \, \hat{\rho} \, | x \rangle \, . \tag{3.6}$$

We can prove the same to the momentum space wave function, i.e.

$$\int dp\, f_w(x,p) = |\tilde{\psi}(p)|^2 = \langle p|\,\hat{\rho}\,|p\rangle\ . \tag{3.7}$$

Using the definition of Eq. (3.2) for the Wigner function from momentum space representation, we prove it by

$$\begin{aligned}\int dx\, f_w(x,p) &= (2\pi\hbar)^{-1}\int_{-\infty}^{\infty} dx\, dk\ \langle p-\frac{k}{2}|\,\hat{\rho}\,|p+\frac{k}{2}\rangle\, e^{\frac{ikx}{\hbar}}\\ &= \int_{-\infty}^{\infty} dk\ \langle p-\frac{k}{2}|\,\hat{\rho}\,|p+\frac{k}{2}\rangle\left[(2\pi\hbar)^{-1}\int dx\, e^{\frac{ikx}{\hbar}}\right]\\ &= \int_{-\infty}^{\infty} dk\ \langle p-\frac{k}{2}|\,\hat{\rho}\,|p+\frac{k}{2}\rangle\ \delta(k) = \langle p|\,\hat{\rho}\,|p\rangle\ .\end{aligned} \tag{3.8}$$

We also require the normalization of Wigner function, through the relation

$$\int f_w(x,p)\, dp\, dx = \mathrm{Tr}\,\hat{\rho} = 1\,. \tag{3.9}$$

To see that this is indeed the case, we start from Eq. (3.1)

$$\int dpdx\, f_w(x,p) = (2\pi\hbar)^{-1}\int dy\, dp\, dx\ \langle x-\frac{y}{2}|\,\hat{\rho}\,|x+\frac{y}{2}\rangle\ e^{\frac{ipy}{\hbar}}\,, \tag{3.10}$$

and then calculate the integral in p:

$$\begin{aligned}\int dpdx\, f_w(x,p) &= \int dy\, dx\ \langle x-\frac{y}{2}|\,\hat{\rho}\,|x+\frac{y}{2}\rangle\ \delta(y)\\ &= \int dx\ \langle x|\,\hat{\rho}\,|x\rangle = \mathrm{Tr}\,\hat{\rho}\,.\end{aligned} \tag{3.11}$$

Finally, we can also prove that Wigner function is not necessarily positive definite following the argument that, if we have $f_\alpha(x,p)$ and $f_\beta(x,p)$ associated

with density matrices $\hat{\rho}_\alpha = |\alpha\rangle\langle\alpha|$ and $\hat{\rho}_\beta = |\beta\rangle\langle\beta|$, we have that

$$\begin{aligned}(2\pi\hbar)^{-1}\int dxdp\, f_\alpha f_\beta &= (2\pi\hbar)^{-2}\int dx\,dp\int dy\,\langle x-\frac{y}{2}|\,\alpha\rangle\langle\alpha\,|x+\frac{y}{2}\rangle\, e^{\frac{ipy}{\hbar}}\\ &\quad\times\int dz\,\langle x-\frac{z}{2}|\,\beta\rangle\langle\beta\,|x+\frac{z}{2}\rangle\, e^{\frac{ipz}{\hbar}}\\ &= (2\pi\hbar)^{-1}\int dx\int dy\,\langle x-\frac{y}{2}|\,\alpha\rangle\langle\alpha\,|x+\frac{y}{2}\rangle\\ &\quad\times\int dz\,\langle x-\frac{z}{2}|\,\beta\rangle\langle\beta\,|x+\frac{z}{2}\rangle\,\delta(y+z)\\ &= (2\pi\hbar)^{-1}\int dx\,dy\,\langle x-\frac{y}{2}|\,\alpha\rangle\langle\alpha\,|x+\frac{y}{2}\rangle\\ &\quad\times\langle x+\frac{y}{2}|\,\beta\rangle\langle\beta\,|x-\frac{y}{2}\rangle\,. \end{aligned}\tag{3.12}$$

Cancelling the $(2\pi\hbar)^{-1}$ factors in both sides and making the change of variables

$$\bar{x} = x-\frac{y}{2}\,,\qquad \bar{y} = x+\frac{y}{2}\,,\tag{3.13}$$

which has Jacobian equal to unity, we obtain:

$$\int dxdp\, f_\alpha f_\beta \;=\; \int d\bar{x}d\bar{y}\,\langle\bar{x}|\,\alpha\rangle\langle\alpha\,|\bar{y}\rangle\,\langle\bar{y}|\,\beta\rangle\langle\beta\,|\bar{x}\rangle = \langle\alpha|\beta\rangle\langle\beta|\alpha\rangle = |\langle\alpha|\beta\rangle|^2\,.\tag{3.14}$$

The right side is positive or zero (orthogonal states). In either case, there is no need for the integrands on the left hand side to be positive in the entire integration range. Therefore, Wigner functions can, in principle have negative values for some values of their arguments; we will provide an example of such a case. The meaning of this is that a Wigner function cannot be called "distribution density", instead, we shall call it "quasi-distribution density" by the properties of Eq. (3.4), (3.7) and (3.9). We can summarize all these properties as follows:

1. $\int f_w(x,p)\,dp = |\psi(x)|^2 = \langle x|\,\hat{\rho}\,|x\rangle\,.$
2. $\int f_w(x,p)dx = |\tilde{\psi}(p)|^2 = \langle p|\,\hat{\rho}\,|p\rangle\,.$
3. $\int f_w(x,p)\,dp\,dx = \mathrm{Tr}\,\hat{\rho} = 1.$
4. f_w is not necessarily positive-definite.

3.1.2 Gaussian Wave Packet Wigner Function

As an example, it is useful to work out the Wigner function for pure states. For such a state, Eq. (3.1) takes the form

$$f_w = (2\pi\hbar)^{-1}\int_{-\infty}^{\infty} dy\, \psi\Big(x-\frac{y}{2}\Big)\psi^*\Big(x+\frac{y}{2}\Big)e^{\frac{ipy}{\hbar}}\,, \tag{3.15}$$

where it is understood that $\psi(x) = \langle x|\psi\rangle$. If ψ is a Gaussian wave packet of form

$$\psi(X) = \Big(\frac{1}{2\pi a^2}\Big)^{\frac{1}{4}} e^{-\frac{X^2}{4a^2}}\,, \tag{3.16}$$

we can make $X = x \pm y/2$ in the exponential; the Wigner function of this wave packet takes the form

$$\begin{aligned} f_w(x,p) &= \frac{1}{2\pi\hbar\sqrt{2\pi a^2}}\int_{-\infty}^{\infty} dy\, e^{-\frac{x^2}{4a^2}} e^{+\frac{xy}{2a^2}} e^{-\frac{y^2}{16a^2}} e^{-\frac{x^2}{4a^2}} e^{-\frac{xy}{2a^2}} e^{-\frac{y^2}{16a^2}} e^{\frac{ipy}{\hbar}} \\ &= \frac{e^{-\frac{x^2}{2a^2}}}{2\pi\hbar\sqrt{2\pi a^2}}\int_{-\infty}^{\infty} dy\, e^{\frac{ipy}{\hbar}-\frac{y^2}{8a^2}} \\ &= \frac{1}{\pi\hbar}\, e^{-\frac{x^2}{2(\Delta x)^2}}\, e^{-\frac{p^2}{2(\Delta p)^2}}\,. \end{aligned} \tag{3.17}$$

The values of root mean square half-widths of the position and momentum distribution $\Delta x = a$ and $\Delta p = \frac{\hbar}{2a}$ were used to explicit the symmetry between x and p. The most general Gaussian wave function is obtained by displacing the center of the state to an arbitrary point in phase space, $\Delta x = x_0$ and $\Delta p = p_0$

$$\psi(x) = (2\pi a^2)^{-\frac{1}{4}}\, e^{-\frac{(x-x_0)^2}{4a^2}}\, e^{\frac{ip_0 x}{\hbar}}\,, \tag{3.18}$$

so

$$f_w(x,p) = \frac{1}{\pi\hbar}\, e^{-\frac{(x-x_0)^2}{2(\Delta x)^2}}\, e^{-\frac{(p-p_0)^2}{2(\Delta p)^2}}\,. \tag{3.19}$$

Note that this is the product of position and momentum distribution, and it is positive everywhere. It has been proven in Ref. [54] that Gaussian wave functions are the only pure states with non-negative Wigner functions. We can see the shape of such function in Figure 3.1.

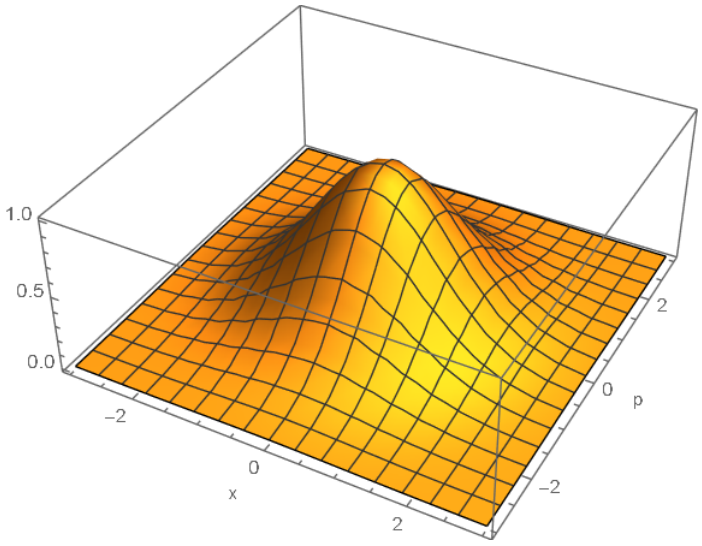

Figure 3.1: Wigner function for Gaussian wave packet

3.1.3 Two Separated Gaussian Wave Packets Wigner Functions

In the case of two separated Gaussian wave packets, considering their superposition and the packets centered in $x = \pm c$ (c is an arbitrary real number):

$$\psi(x) = \frac{N}{\sqrt{2}(2\pi a^2)^{\frac{1}{4}}}\left[e^{-\frac{(x-c)^2}{4a^2}} + e^{-\frac{(x+c)^2}{4a^2}}\right]. \tag{3.20}$$

The normalization factor $N = (1 + e^{\frac{-c^2}{2a^2}})^{-\frac{1}{2}}$ is required because the Gaussians are not orthogonal. When we evaluate Wigner function from Eq. (3.15) there will be two separate Gaussian packets and one interference term. The result is

$$f_w(x,p) = \frac{N^2}{2\pi\hbar}\, e^{\frac{-p^2}{2(\Delta p)^2}}\left[e^{-\frac{(x-c)^2}{2(\Delta x)^2}} + e^{-\frac{(x+c)^2}{2(\Delta x)^2}}\right] + \frac{N^2}{2\pi\hbar}\, e^{\frac{-p^2}{2(\Delta p)^2}}\, e^{-\frac{x^2}{2(\Delta x)^2}} \cos\frac{2cp}{\hbar}. \tag{3.21}$$

In this expression we used $\Delta x = a$ and $\Delta p = \frac{\hbar}{2a}$. We can see the previous peak at $x = \pm c$ and another one at $x = 0$. It is worth noting that we have the previous Gaussian Wigner function multiplied by an oscillatory factor that represents interference between the two Gaussian wave packets we are now dealing with. Clearly this Wigner function takes both positive and negative values, and cannot be interpreted as a probability distribution, and we also have the fact that it retains this character even in the macroscopic limit in which the separation c between the packets becomes infinitely large because, as $c \to \infty$, the amplitude of the interference term does not diminish. This Wigner function does not approach

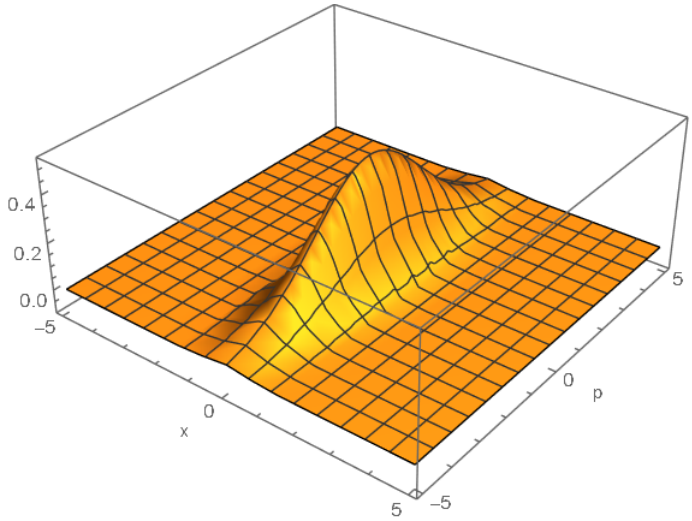

Figure 3.2: Wigner function for the wave packet in Eq. (3.20) for $c = 0$.

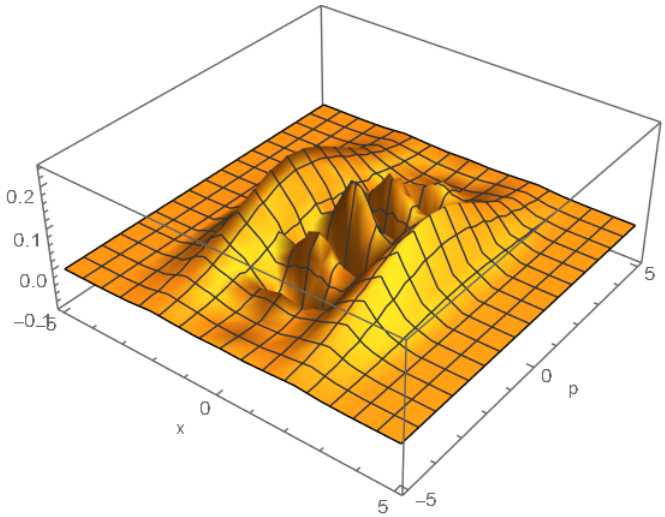

Figure 3.3: Same as in Fig. 3.2, for $c = 2$.

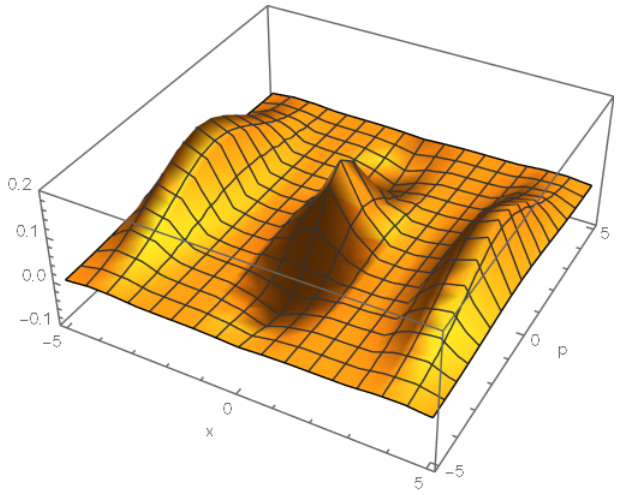

Figure 3.4: Same as in Fig. 3.2, for $c = 4$.

a classical phase space probability distribution even in the macroscopic limit (see Figures 3.2, 3.3, 3.4 and 3.5), but it does not prevent it from yielding the expected two-peak position distribution, since the interference term averages to zero upon integration over momentum.

3.1.4 Time Evolution of Wigner Function

Since Wigner function is the Fourier transform of density matrix, time evolution of the former can be reduced to that of the later. Considering the Hamiltonian of form $H = \frac{P^2}{2m} + V$ (with capital P to avoid confusion), its time evolution in Heisenberg picture is given by:

$$\frac{d\rho(t)}{dt} = \frac{i}{\hbar}\Big[\rho(t), H(t)\Big]\,. \tag{3.22}$$

It is convenient to separate the time evolution of density matrix as

$$\frac{d\rho}{dt} = \frac{\partial\rho_K}{\partial t} + \frac{\partial\rho_V}{\partial t}\,, \tag{3.23}$$

where ρ_K is the kinetic part and ρ_V is the potential one. The kinetic term then becomes

$$\frac{\partial\rho_K}{\partial t} = \frac{i}{2m\hbar}(\rho P^2 - P^2\rho)\,, \tag{3.24}$$

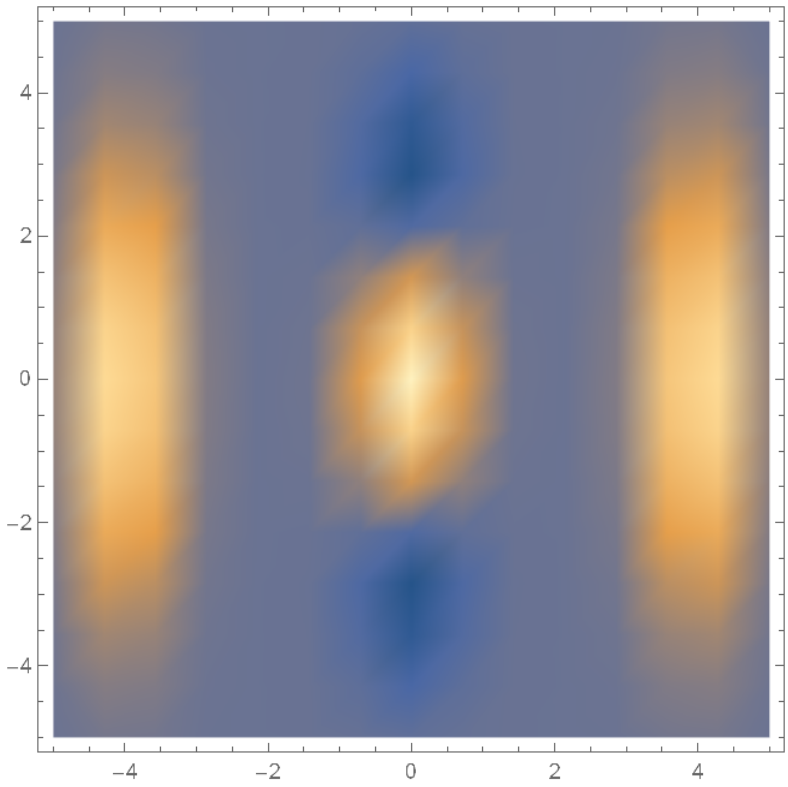

Figure 3.5: Wigner function horizontal cut from Figure 3.4, with negative values in deep blue.

and the potential one

$$\frac{\partial \rho_V}{\partial t} = \frac{i}{\hbar}(\rho V - V\rho)\,. \tag{3.25}$$

We use the momentum representation to evaluate the kinetic part:

$$\begin{aligned}\frac{\partial \rho_K}{\partial t}\langle p|\,\rho\,|p'\rangle &= \frac{i}{2m\hbar}\langle p|\,\rho\,|p'\rangle\,(p'^2 - p^2)\\ &= \frac{i}{2m\hbar}\langle p|\,\rho\,|p'\rangle\,(p'-p)(p'+p)\,,\end{aligned} \tag{3.26}$$

and the Wigner function definition of Eq. (3.2) to find

$$\frac{\partial f_{w(k)}(x,p;t)}{\partial t} = \frac{i}{\hbar m}\int_{-\infty}^{\infty} dk\, p\, k\ \langle p - \frac{k}{2}|\,\rho\,|p + \frac{k}{2}\rangle\, e^{\frac{ixk}{\hbar}}\,. \tag{3.27}$$

Now we replace the k inside the integral for $(-\hbar/i)\frac{\partial}{\partial x}$ and take it off the integral

$$\frac{\partial f_{w(k)}(x,p;t)}{\partial t} = -\frac{p}{m}\frac{\partial}{\partial x} f_w(x,p,t)\,. \tag{3.28}$$

In the non-kinetic term case, the time evolution in position representation given by Eq. (3.1) is

$$\frac{\partial}{\partial x}\langle x|\,\rho_V\,|x'\rangle = \frac{i}{\hbar}\langle x|\,\rho\,|x'\rangle\left[V(x) - V(x')\right]. \tag{3.29}$$

Using the Wigner transformation definition in we obtain

$$\frac{\partial}{\partial t} f_{w(V)}(x,p;t) = \frac{i}{\hbar(2\pi\hbar)}\int_{-\infty}^{\infty} dy\ \langle x - \frac{y}{2}|\,\rho\,|x + \frac{y}{2}\rangle\left[V\Big(x+\frac{y}{2}\Big) - V\Big(x-\frac{y}{2}\Big)\right] e^{\frac{ipy}{\hbar}}\,. \tag{3.30}$$

If $V(x)$ is analytic it can be expressed as a Taylor series:

$$V\Big(x+\frac{y}{2}\Big) - V\Big(x-\frac{y}{2}\Big) = \sum_{n=odd}\frac{2}{n!}\Big(\frac{y}{2}\Big)^n\frac{d^nV(x)}{dx^n}\,. \tag{3.31}$$

When we use this series expansion in the integral, we can replace the term $(\frac{1}{2}y)^n$ for $\Big(-\frac{\hbar}{2i}\frac{\partial}{\partial x}\Big)^n$ which yields

$$\frac{\partial f_{w(V)}(x,p,t)}{\partial t} = \sum_{n=odd}\frac{1}{n!}\Big(-\frac{i\hbar}{2}\Big)^{n-1}\frac{d^nV(x)}{dx^n}\frac{\partial^n}{\partial p^n} f_w(x,p,t)\,. \tag{3.32}$$

The sum of these two equations amounts to the time evolution of Wigner function.

There are some aspects to emphasize: first, the complex number i appears with

even power, so all terms are real; second, this sum is evidently a sum of powers of $\hbar$, which suggests this equation has a neat classical limit. Combining the two kinetic and potential parts we obtain

$$\frac{\partial f_w(x,p;t)}{\partial t} = -\frac{p}{m}\frac{\partial}{\partial x} f_w(x,p;t) + \frac{dV(x)}{dx}\frac{\partial}{\partial p} f_w(x,p;t) + \mathcal{O}(\hbar^2)\,. \tag{3.33}$$

If the corrections of $\mathcal{O}(\hbar^2)$ can be neglected, this is the classical Liouville equation:

$$\frac{\partial \rho(x,p;t)}{\partial t} = -\frac{p}{m}\frac{\partial}{\partial q}\rho(x,p;t) - F(q)\frac{\partial}{\partial p}\rho(x,p;t)\,. \tag{3.34}$$

The corrections terms, formally of order $\hbar^n$ involve a nth order derivative of $f_w(x,p;t)$ with respect to p, so this can generate factors of $1/\hbar$ and cancel the $\hbar$ factors. Equation (3.21) is an example of Wigner function that behaves this way (see Figure 3.5). In such cases the corrections terms in Eq. (3.33) do not vanish in the $\hbar \to 0$ limit.

The harmonic oscillator is an interesting case; since the third and higher derivatives of $V(x)$ vanish (due to the quadratic potential), the terms in the Eq. (3.32) for $n > 1$ (which contain $\hbar$) are all 0. Hence its Wigner function satisfies the classical Liouville equation exactly, even if the state is not nearly classical.

3.1.5 Quantum Entropy in Wigner Representation

The Wigner function provides a bridge between quantum and classical phase-space physics. In particular, the fact that the Wigner function be negative motivates its use to quantify quantum entanglement, the quintessential quantum property. Quantum entanglement plays a fundamental role in quantum information science. A key concept in quantifying entanglement is entanglement entropy. We cannot dwell much into this subject, but these feature motivate us to compute a quantum entropy in quantum field theory using the Wigner functional approach developed in this work. In the following we present a brief outline of the main results we need to compute a quantum entropy.

One of the most studied quantum entropies is the von Neumann entropy $S_{\rm vN}$, also known as the entanglement entropy. It is defined in terms of the density matrix $\hat{\rho}$ by [55]:

$$S_{\rm vN} = -\operatorname{Tr}\hat{\rho}\ln\hat{\rho}\,. \tag{3.35}$$

The von Newman extropy provides a quantitative measure of the information

available on a system's state described by $\hat{\rho}$. The larger $S_{\rm vN}$, the less the available information. If $\hat{\rho}$ is a pure state, i.e. the state of the system is described by state vector, we have complete knowledge on the state and, therefore $S_{\rm vN} = 0$. On the other hand, if $\hat{\rho}$ describes a mixed state, $S_{\rm vN} \geq 0$.

One obtains the classical limit (CL) of the Von Neumann entropy by replacing the density matrix with the phase-space probability distribution $f(x,p)$:

$$S_{\rm vN} \xrightarrow{\rm CL} \int dxdp\, f(x,p) \ln f(x,p)\,. \tag{3.36}$$

Although appealing, one cannot replace $f(x,p)$ by $f_w(x,p)$ to obtain a well defined quantum entropy functional because $f_w(x,p)$ can take negative values. However, one can still define a quantum entropy in terms of the Wigner function $f_w(x,p)$ as [56]:

$$S_w = 1 - 2\pi\hbar \int dxdp\, f_w^2\,. \tag{3.37}$$

S_w was denoted S_2 in Ref. [56]. This entropy is equal to the linear entropy, which is given in terms of $\hat{\rho}$ by:

$$S_L = 1 - {\rm Tr}\,\rho^2\,. \tag{3.38}$$

To prove this, we first use the definition of $f_w(x,p)$ and write:

$$\begin{aligned}
(2\pi\hbar)\int f_w^2(x,p)dxdp &= (2\pi\hbar)^{-1}\int dx\,dp\,\Big(\int_{-\infty}^{\infty} dy\,\langle x-\frac{y}{2}|\,\rho\,|x+\frac{y}{2}\rangle\, e^{\frac{ipy}{\hbar}}\Big) \\
&\quad\times\Big(\int_{-\infty}^{\infty} dy'\,\langle x-\frac{y'}{2}|\,\rho\,|x+\frac{y'}{2}\rangle\, e^{\frac{ipy'}{\hbar}}\Big) \\
&= \int dx\Big(\int_{-\infty}^{\infty} dy\;\langle x-\frac{y}{2}|\,\rho\,|x+\frac{y}{2}\rangle\Big) \\
&\quad\times\Big(\int_{-\infty}^{\infty} dy'\;\langle x-\frac{y'}{2}|\,\rho\,|x+\frac{y'}{2}\rangle\Big)\,\delta(y+y') \\
&= \int dx\,dy\;\langle x-\frac{y}{2}|\,\rho\,|x+\frac{y}{2}\rangle\,\langle x+\frac{y}{2}|\,\rho\,|x-\frac{y}{2}\rangle\;.
\end{aligned} \tag{3.39}$$

Then we change variables as

$$u = x - \frac{y}{2} \quad \text{and} \quad v = x + \frac{y}{2}\,. \tag{3.40}$$

Since the Jacobian of the transformation is unity, we obtain

$$\int du\, dv\ \langle u|\,\rho\,|v\rangle\,\langle v|\,\rho\,|u\rangle = \int du\,\langle u|\,\rho\rho\,|u\rangle = \mathrm{Tr}\,\rho^2\,, \tag{3.41}$$

and $S_w = S_L$ is verified.

In the quantum field theory literature associated with quantum information concepts it is common to work with the n^{th} Rényi entropies [55]:

$$S_n = \frac{1}{1-n}\ln \mathrm{Tr}\,\hat{\rho}^n. \tag{3.42}$$

The von Neuman entropy is then obtained from the S_n through the replica trick formula:

$$S_{\text{vN}} = \lim_{n\to 1} S_n\,. \tag{3.43}$$

The reason for the use of S_n is that it is almost impossible to compute S_{vN} in practice directly from $\hat{\rho}$, because one would need to diagonalize $\hat{\rho}$ to be able to compute its logarithm.

Now, it is important to notice that S_2 is the only Rényi entropy that has the $\hat{\rho} \leftrightarrow f_w$ correspondence. For example, $\mathrm{Tr}\,\hat{\rho}^4$ does not correspond to $\int dxdp\, f_w^4(x,p)$. For this reason, in this dissertation we will compute the 2^{nd} Rényi entropy:

$$S_2 = -\ln \mathrm{Tr}\,\hat{\rho}^2\,. \tag{3.44}$$

To conclude this section, we illustrate the computation of S_w for the one-dimensional Wigner function in Eq. (3.1) of a Gaussian wave packet (with minimum uncertainty):

$$f_w(x,p) = \frac{1}{\pi\hbar}\, e^{\frac{-x^2}{2(\Delta x)^2}}\, e^{\frac{-p^2}{2(\Delta p)^2}}\,, \tag{3.45}$$

where Δx and Δp are the half widths of the Gaussian distributions and obey $\Delta x \Delta p = \hbar/2$, and are independent of x and p. The S_w entropy for this case is computed as follows:

$$\begin{aligned} S_w &= 1 - \pi\hbar \int \frac{1}{\pi^2\hbar^2} e^{\frac{-x^2}{(\Delta x)^2}} e^{\frac{-p^2}{(\Delta p)^2}}\, dxdp \\ &= 1 - \frac{2\pi\hbar}{\pi^2\hbar^2}\left(\int e^{\frac{-x^2}{(\Delta x)^2}} dx\right)\left(\int e^{\frac{-p^2}{(\Delta p)^2}} dp\right) \\ &= 1 - \frac{2}{\pi\hbar}\left(\sqrt{\pi}\Delta x\right)\left(\sqrt{\pi}\Delta p\right) = 1 - \frac{2\Delta x\Delta p}{\hbar} = 0\,. \end{aligned} \tag{3.46}$$

Here, we have used that $\Delta x \Delta p = \hbar/2$. The null result is due to the pure-state nature of the f_w used; we recall that pure-state density matrix $\hat{\rho}$ has the property $\hat{\rho}^2 = \hat{\rho}$. Note $S_w = 0$ is a necessary condition for the state represented by f_w being pure; it is not a sufficient condition because one can find counterexamples for which $S_w = 0$ for a non pure state [56].

3.2 Wigner Functional Approach to Quantum Field Theory

In this section we review the previous formalism to field theory following the work of Mrówczyński and Müller in Ref. [11] for a scalar quantum field theory. The generalization to the electromagnetic field is presented in Ref. [13] and to the fermion fields in Ref. [25].

We begin by defining a "Wigner Functional" in phase space as

$$\begin{aligned} W[\Phi(x), \Pi(x); t] &= \int D\varphi(x)\, e^{-i\int dx\, \Pi(x)\varphi(x)} \\ &\quad \times \left\langle \Phi(x) + \frac{\varphi(x)}{2} \middle| \hat{\rho}(t) \middle| \Phi(x) - \frac{\varphi(x)}{2} \right\rangle . \end{aligned} \tag{3.47}$$

In momentum space, we know from the previous chapter that $\Phi(p)$ and $\Pi(p)$ are now complex numbers and their real and imaginary parts are not independent of each other anymore due to the constrain $\Phi^*(p) = \Phi(-p)$. To avoid double counting of degrees of freedom, the real and imaginary parts of these fields are treated as independent variables in the path integral, but with the momentum restricted to positive values ($p \geq 0$). The Wigner functional in terms of momentum space fields can then be defined by

$$\begin{aligned} \widetilde{W}[\Phi(p), \Pi(p); t] &= \int D\varphi(p) e^{-i\int_0^\infty \frac{dp}{2\pi}\, [\Pi^*(p)\varphi(p) + \Pi(p)\varphi^*(p)]} \\ &\quad \times \left\langle \Phi(p) + \frac{\varphi(p)}{2} \middle| \hat{\rho}(t) \middle| \Phi(p) - \frac{\varphi(p)}{2} \right\rangle , \end{aligned} \tag{3.48}$$

where $D\varphi(p)$ means integration over the real and imaginary parts of $\varphi(p)$, and the transformation from coordinate to momentum space is done by a Fourier transform with unit Jacobian:

$$\det \left[\frac{\delta\Phi(x)}{\delta\Phi(p)} \right] = 1 . \tag{3.49}$$

3.2.1 Expectation Values

We can define the expectation value of an operator $\hat{\mathcal{O}}(\hat{\Phi}, \hat{\Pi})$ as

$$\langle \hat{\mathcal{O}}(\hat{\Phi}, \hat{\Pi}) \rangle = \frac{1}{\mathrm{Tr}\, \hat{\rho}(t)} \mathrm{Tr} \left[\hat{\rho}(t)\, \hat{\mathcal{O}}(\hat{\Phi}, \hat{\Pi} \right] = \frac{1}{Z} \mathrm{Tr} \left[\hat{\rho}(t)\, \hat{\mathcal{O}}(\hat{\Phi}, \hat{\Pi} \right] , \tag{3.50}$$

where we defined

$$Z \equiv \mathrm{Tr}\ \hat{\rho}(t) = \int D\Phi \frac{D\Pi}{2\pi} W[\Phi, \Pi; t] \, . \tag{3.51}$$

We prove in Appendix C that

$$\langle \hat{\mathcal{O}}(\hat{\Phi}, \hat{\Pi}) \rangle = \frac{1}{Z} \int D\Phi \frac{D\Pi}{2\pi} \mathcal{O}(\Phi, \Pi)\, W[\Phi, \Pi; t] \, , \tag{3.52}$$

provided that the non-commuting operators in $\mathcal{O}$ are properly symmetrized. Every operator corresponding to an asymmetric ordering of the operators $\hat{\Phi}$ and $\hat{\Pi}$ must be explicitly expressed as sums of symmetrized factors. Wigner functional in the previous expression looks like a probability density in statistical mechanics, but like the Wigner function case, it might not be positive definite, termed a "quasi-distribution" functional.

A warning on the the meaning of quantities denoted by Z is necessary before we proceed: Z means different quantities in different places in this work. In the previous chapter we used Z to denote generating functional, here we used to denote the trace of the density matrix, and shortly ahead we use Z to denote thermal partition functions.

3.2.2 Equation of Motion

We know from Ref. [42], for example, that density matrix obey the dynamical equation

$$i\hbar \frac{d}{dt} \hat{\rho}(t) = \left[\hat{H}, \hat{\rho}(t) \right] , \tag{3.53}$$

and from Section 2.2 we know that for a scalar field theory we have a Hamiltonian of the form

$$\hat{H} = \int dx \left[\frac{1}{2} \left(\hat{\Pi}^2(x) + (\nabla \hat{\Phi}(x))^2 + m^2 \hat{\Phi}^2(x) \right) - \mathcal{L}_I(\hat{\Phi}) \right] , \tag{3.54}$$

where $\hat{\Pi}$ is the conjugated momentum. We derive in Appendix C.2 the equation of motion for this Hamiltonian as being

$$\frac{\partial}{\partial t}W[\Phi,\Pi,t] \;+\; \int dx\Bigg[\Pi(x)\frac{\delta}{\delta\Phi(x)} - \Big(m^2\Phi(x)-\nabla^2\Phi(x)\Big)\frac{\delta}{\delta\Pi(x)} + \mathcal{K}_I(x)\Bigg]W[\Phi,\Pi,t] = 0\,, \tag{3.55}$$

where

$$\mathcal{K}_I(x) = -\frac{i}{\hbar}\mathcal{L}_I\left[\Phi(x)+\frac{i\hbar}{2}\frac{\delta}{\delta\Pi(x)}\right] + \frac{i}{\hbar}\mathcal{L}_I\left[\Phi(x)-\frac{i\hbar}{2}\frac{\delta}{\delta\Pi(x)}\right]. \tag{3.56}$$

In the $\mathcal{L}_I(x) = -\frac{\lambda}{4!}\Phi^4(x)$ case:

$$\mathcal{K}_I(x) = \frac{\lambda}{6}\left[-\Phi^3(x)\frac{\delta}{\delta\Pi(x)} + \frac{\hbar^2}{4}\Phi(x)\frac{\delta^3}{\delta\Pi^3(x)}\right]. \tag{3.57}$$

We note that this interaction term $\mathcal{K}_I$ is always finite for renormalizable quantum field theories in $(3+1)$ spacetime dimensions because their Lagrangians contain at most quartic terms in the interaction. This equation has the suggestive form of a transport equation and can be written in the form of a classical Liouville equation [44] when neglecting higher derivative terms

$$\left[\frac{\partial}{\partial t} + \int dx\left(\frac{\delta H}{\delta\Pi(x)}\frac{\delta}{\delta\Phi(x)} - \frac{\delta H}{\delta\Phi(x)}\frac{\delta}{\delta\Pi(x)}\right)\right]W[\Phi,\Pi,;t] = 0\,, \tag{3.58}$$

where the neglected terms are of order $\hbar^2$ or higher, showing us that quantum corrections are of orders of $\hbar$ for this specific case, but not for all [53].

3.2.3 Free Field in Thermal Equilibrium

We will consider a scalar field in thermodynamical equilibrium at some temperatue T; the corresponding density matrix is given by

$$\hat{\rho}_\beta^{(0)} = \frac{1}{Z^{(0)}}\,e^{-\beta\hat{H}_0}\,, \tag{3.59}$$

where $\beta = 1/T$ (we take the Boltzmann constant equal to unity). $Z^{(0)}$ is the partition function, given by

$$Z^{(0)} = \mathrm{Tr}\,e^{-\beta\hat{H}_0}\,, \tag{3.60}$$

so that the thermal density matrix is normalized to unity:

$$\mathrm{Tr}\,\hat{\rho}^{(0)} = 1\,. \tag{3.61}$$

The superscript (0) in $\hat{\rho}_\beta^{(0)}$ and $Z^{(0)}$ indicates that it corresponds to the Hamiltonian $\hat{H}_0$ of Eq. (3.64). In the following we will use the superscript (0) in all quantities referring to $\hat{H}_0$ to avoid confusion when changing to other Hamiltonians. We shall also suppress from now on the time in the equations since we are dealing with statistical mechanics under thermal equilibrium. Note that for a real scalar field there is no conserved charge and thus no chemical potential (this is similar to a gas of photons, but the particles here have a mass).

It is convenient to work in momentum space. In order to find the momentum space version of Hamiltonian of Eq. (3.54) we first Fourier transform each term explicitly

$$\begin{aligned}
\frac{1}{2}\int dx \hat{\Pi}^2(x) &= \frac{1}{2}\int dx \left[\int_{-\infty}^{\infty}\frac{dp}{2\pi}\hat{\Pi}(p)\,e^{-ipx}\right]\left[\int_{-\infty}^{\infty}\frac{dq}{2\pi}\hat{\Pi}(q)\,e^{-iqx}\right] \\
&= \frac{1}{2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{dpdq}{2\pi 2\pi}\,\hat{\Pi}(p)\,\hat{\Pi}(q)\int dx\,e^{-i(p+q)x} \\
&= \frac{1}{2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{dpdq}{2\pi 2\pi}\hat{\Pi}(p)\hat{\Pi}(q)\,2\pi\,\delta(p+q) \\
&= \frac{1}{2}\int_{-\infty}^{\infty}\frac{dp}{2\pi}\,\hat{\Pi}(p)\,\hat{\Pi}(-p) = \frac{1}{2}\int_{-\infty}^{\infty}\frac{dp}{2\pi}\,\hat{\Pi}^\dagger(p)\,\hat{\Pi}(p)\,,
\end{aligned} \tag{3.62}$$

where we used the fact that Π and $\Pi^\dagger$ commute. Likewise for the $\hat{\Phi}$ terms:

$$\frac{1}{2}\int dx\left[(\nabla\hat{\Phi}(x))^2 + m^2\Phi^2(x)\right] = \frac{1}{2}\int_{-\infty}^{\infty}\frac{dp}{2\pi}\left(p^2+m^2\right)\,\hat{\Phi}^\dagger(p)\hat{\Phi}(p)\,, \tag{3.63}$$

then we finally glue together Eqs. (3.62) and (3.63):

$$\hat{H}_0 = \frac{1}{2}\int_{-\infty}^{\infty}\frac{dp}{2\pi}\left[\hat{\Pi}^\dagger(p)\hat{\Pi}(p) + (p^2+m^2)\hat{\Phi}^\dagger(p)\hat{\Phi}(p)\right]. \tag{3.64}$$

We show in Appendix C that we can write the Wigner functional for this case as

$$\widetilde{W}_\beta^{(0)}[\Phi,\Pi] = C_\beta\,\exp\left\{-\frac{\beta}{2}\int_{-\infty}^{\infty}\frac{dp}{2\pi}\,\tilde{\Delta}_\beta(p)\left[\Pi^*(p)\Pi(p) + E^2(p)\Phi^*(p)\Phi(p)\right]\right\}, \tag{3.65}$$

where $E(p) = \sqrt{p^2 + m^2}$ and the thermal weight factor

$$\tilde{\Delta}_\beta(p) = \frac{2}{\beta E(p)} \tanh \frac{\beta E(p)}{2} . \tag{3.66}$$

The normalization is

$$C_\beta = \exp\left[L \int_{-\infty}^{\infty} \frac{dp}{2\pi} \ln\left(2 \tanh \frac{\beta E(p)}{2} \right) \right] , \tag{3.67}$$

where L is the quantization volume (in this case in one-dimension).

In the high temperature limit we have $\tilde{\Delta}_\beta(p) \to 1$ and we reproduce the classical limit

$$\widetilde{W}_\beta^{cl}(\Phi, \Pi) = \exp\Big\{ -\frac{\beta}{2} \int_{-\infty}^{\infty} \frac{dp}{2\pi} \Big[\Pi^*(p)\Pi(p) + E^2(p)\Phi^*(p)\Phi(p) \Big] \Big\} . \tag{3.68}$$

We recognize that in this case the Wigner functional depends only on the total energy of the system.

Now we can evaluate the correlation function $\langle \hat{\Phi}^\dagger(p)\hat{\Phi}(p) \rangle$ using the definition of Eq. (3.50) and Wigner functional in Eq. (3.65):

$$\begin{aligned} \langle \hat{\Phi}^\dagger(p)\hat{\Phi}(p) \rangle_0 &= \frac{1}{Z^{(0)}} \int D\Phi \frac{D\Pi}{2\pi} \, \Phi^*(p)\Phi(p) \, W_\beta^{(0)}(\Phi, \Pi) \\ &= \frac{1}{Z_\Pi^{(0)} Z_\Phi^{(0)}} \int D\Phi \frac{D\Pi}{2\pi} \, \Phi^*(p)\Phi(p) \, W_\beta^{(0)}(\Phi) \, W_\beta^{(0)}(\Pi) \\ &= \frac{1}{Z_\Phi^{(0)}} \int D\Phi \, \Phi^*(p)\Phi(p) \, W_\beta^{0}(\Phi) , \end{aligned} \tag{3.69}$$

where

$$Z_\Phi^{(0)} = \int D\Phi \, W_\beta^{(0)}(\Phi) \qquad \text{and} \qquad Z_\Pi^{(0)} = \int \frac{D\Pi}{2\pi} \, W_\beta^{(0)}(\Pi) , \tag{3.70}$$

with

$$\begin{aligned} W_\beta^{(0)}(\Phi) &= \sqrt{C_\beta} \exp\Big\{ -\frac{\beta}{2} \int_{-\infty}^{\infty} \frac{dp}{2\pi} \, \tilde{\Delta}_\beta(p) \, E^2(p) \, \Phi^*(p) \, \Phi(p) \Big\} , \\ W_\beta^{(0)}(\Pi) &= \sqrt{C_\beta} \exp\Big\{ -\frac{\beta}{2} \int_{-\infty}^{\infty} \frac{dp}{2\pi} \, \tilde{\Delta}_\beta(p) \, \Pi^*(p) \, \Pi(p) \Big\} . \end{aligned} \tag{3.71}$$

Therefore, as shown step by step in Appendix C, the correlation function is

given by

$$\langle\hat{\Phi}^{\dagger}(p)\hat{\Phi}(p)\rangle_0 = \frac{L}{2E(p)\tanh\frac{\beta E(p)}{2}} = \frac{L}{E(p)}\left(\frac{1}{e^{\frac{\beta E(p)}{2}}-1}+\frac{1}{2}\right), \tag{3.72}$$

where the last term is a zero temperature contribution. Likewise, we obtain

$$\begin{aligned}\langle\hat{\Pi}^{\dagger}(p)\hat{\Pi}(p)\rangle_0 &= \frac{1}{Z}\int D\Phi\,\frac{D\Pi}{2\pi}\,\Pi^*(p)\Pi(p)\,W(\Phi,\Pi)\\ &= \frac{1}{Z_{\Pi}^{(0)}Z_{\Phi}^{(0)}}\int D\Phi\frac{D\Pi}{2\pi}\,\Pi^*(p)\,\Pi(p)\,W(\Phi)\,W(\Pi)\\ &= \frac{1}{Z_{\Pi}^{(0)}}\int\frac{D\Pi}{2\pi}\,\Pi^*(p)\,\Pi(p)\,W(\Pi)\,,\end{aligned} \tag{3.73}$$

and finally we find

$$\langle\hat{\Pi}^{\dagger}(p)\hat{\Pi}(p)\rangle_0 = \frac{E(p)L}{2\tanh\frac{\beta E(p)}{2}} = E(p)L\left(\frac{1}{e^{\frac{\beta E(p)}{2}}-1}+\frac{1}{2}\right). \tag{3.74}$$

Consequently we conclude that

$$\sqrt{\langle\hat{\Phi}^{\dagger}(p)\hat{\Phi}(p)\rangle_0\,\langle\hat{\Pi}^{\dagger}(p)\hat{\Pi}(p)\rangle_0} = \frac{L}{2\tanh\frac{\beta E(p)}{2}} \geq \frac{L}{2}\,, \tag{3.75}$$

which shows us that the uncertainty picture is built in Wigner functional.

When we know the Wigner functional in momentum space, it is easy to find it in configuration space by Fourier transforming their terms as

$$W_{\beta}^{(0)}[\Phi,\Pi] = C\,\exp\Big[-\beta\int dxdx'\mathcal{H}_0(x,x')\Big]\,, \tag{3.76}$$

where

$$\mathcal{H}_0(x,x') \equiv \frac{1}{2}\Delta_{\beta}(x-x')\Big[\Pi(x)\Pi(x')+\nabla\Phi(x)\nabla\Phi(x')+m^2\Phi(x)\Phi(x')\Big]\,, \tag{3.77}$$

and it is understood that

$$\Delta_{\beta}(x) = \int_{-\infty}^{\infty}\frac{dp}{2\pi}\,e^{-ipx}\,\tilde{\Delta}_{\beta}(p)\,. \tag{3.78}$$

We can see that $\Delta_{\beta}(x)\approx\delta(x)$ for $m^{-1},|x|\gg\beta$ i.e. the classical limit. In the $m=0$

limit this integral can be analytically computed in one dimension, yielding

$$\Delta_\beta(x) = \frac{2}{\beta\pi} \ln\left(\coth\frac{\pi|x|}{2\beta}\right), \tag{3.79}$$

and approximated by the cases

$$\Delta_\beta(x) \approx \begin{cases} \frac{2}{\beta\pi}\ln\frac{|x|}{\beta} & \text{for } |x| \ll \beta\,, \\ \frac{4}{\beta\pi}e^{-\frac{\pi|x|}{\beta}} & \text{for } |x| \gg \beta\ . \end{cases} \tag{3.80}$$

3.2.4 Generating Functional in Phase Space

In this section we define the Generating Functional in phase space as:

$$\begin{aligned} Z[J(x)] &= \int D\Phi\,\frac{D\Pi}{2\pi}\,W(\Phi,\Pi)\,e^{\beta\int dx\,\Phi(x)J(x)} \\ &= \int D\Phi\,\frac{D\Pi}{2\pi}\,e^{-\beta\int dx\,dx'\left[\mathcal{H}(x,x')-\delta(x-x')\Phi(x)J(x')\right]}, \end{aligned} \tag{3.81}$$

where I have used $\mathcal{H}(x,x')$ of Eq. (3.77) and $J(x)$ is some external current. We are now able to rewrite the previous results for the correlation function in a new fashion for phase space, using this generating functional as (see Ref. [11])

$$Z[J(x)] = N\,\exp\left[\frac{\beta}{2}\int dx\,dx'\,J(x)G(x-x')J(x')\right], \tag{3.82}$$

where the propagator is

$$G(x) = \int \frac{dp}{2\pi}\frac{e^{-ipx}}{\tilde{\Delta}_\beta(p)(p^2+m^2)}, \tag{3.83}$$

As showed in previous section, using generating functionals it is easy to evaluate the two-point correlation function:

$$\langle\hat{\Phi}(x)\hat{\Phi}(y)\rangle = \frac{1}{\beta^2}\frac{1}{Z[0]}\frac{\delta^2 Z[J]}{\delta J(y)\delta J(x)}\Big|_{J=0} = G(x-y)\,. \tag{3.84}$$

We can go even further, making use $\tilde{\Delta}_\beta(p)$ of Eq. (3.66) to rewrite the propaga-

tor as

$$\begin{aligned} G(x) &= \int \frac{dp}{2\pi} \frac{\beta E(p) e^{-ipx}}{2E^2(p) \tanh \frac{\beta E(p)}{2}} = \frac{\beta}{2} \int \frac{dp}{2\pi} \frac{e^{-ipx}}{E(p)} \frac{e^{\frac{\beta E(p)}{2}} + e^{-\frac{\beta E(p)}{2}}}{e^{\frac{\beta E(p)}{2}} - e^{-\frac{\beta E(p)}{2}}} \\ &= \frac{\beta}{2} \int \frac{dp}{2\pi} \frac{e^{-ipx}}{E(p)} \frac{e^{\beta E(p)} + 1}{e^{\beta E(p)} - 1} = \frac{\beta}{2} \int \frac{dp}{2\pi} \frac{e^{-ipx}}{E(p)} \left[\frac{2}{e^{\beta E(p)} - 1} + 1 \right] \\ &= \beta \int \frac{dp}{2\pi} \frac{e^{-ipx}}{E(p)} \frac{1}{e^{\frac{\beta E(p)}{2}} - 1} + \frac{\beta}{2} \int \frac{dp}{2\pi} \frac{e^{-ipx}}{E(p)}, \end{aligned} \tag{3.85}$$

where we can clearly see the Bose-Einstein distribution in the first therm, which vanishes in the limit of zero temperature. This integral for the propagator can be evaluated analytically [57] for three dimensions and $m = 0$:

$$G(\mathbf{x}) = \frac{1}{4\pi|\mathbf{x}|} \frac{\sinh(\frac{2\pi|\mathbf{x}|}{\beta})}{\cosh(\frac{2\pi|\mathbf{x}|}{\beta}) - 1}, \tag{3.86}$$

knowing that

$$G(\mathbf{x}) = \begin{cases} \frac{1}{4\pi|\mathbf{x}|} & \text{for } \beta \ll |\mathbf{x}|, \\ \frac{\beta}{4\pi^2|\mathbf{x}|^2} & \text{for } \beta \gg |\mathbf{x}|. \end{cases} \tag{3.87}$$

For a finite mass we can evaluate the propagator integral in an approximate way again for three dimensions:

$$G(\mathbf{x}) = \frac{1}{4\pi|\mathbf{x}|} e^{-m|\mathbf{x}|}. \tag{3.88}$$

If we have $m^{-1} \gg \beta$ and $|\mathbf{x}| \gg \beta$ (which is the classical limit condition):

$$G(\mathbf{x}) \approx \frac{\beta m}{4\pi^2|\mathbf{x}|} \mathbf{K}_1(m|\mathbf{x}|) \approx \frac{\beta\sqrt{m}}{2^{5/2}\pi^{3/2}|\mathbf{x}|^{3/2}} e^{-m|\mathbf{x}|}, \tag{3.89}$$

where the first approximation holds under the assumption of $m^{-1} \ll \beta$, the second requires also $m^{-1} \ll |\mathbf{x}|$.

3.2.5 Mean Field Approximation

In the mean field (MF) approximation for the scalar field we make the substitution

$$\frac{\lambda}{4!}\hat{\Phi}^4(x) \longrightarrow \frac{\lambda}{4}\langle\hat{\Phi}^2(x)\rangle\hat{\Phi}^2(x)\,. \tag{3.90}$$

The combinatorial factor 4! changes to 4 because there are 6 ways to select 2 out of 4 available. This change is pretty convenient since it represents (due to the $\hat{\Phi}^2(x)$ dependence) a "mas term".

It is important to emphasize that the choice for $\langle\Phi^2(x)\rangle$ is the only useful one, since the other ones like $\langle\Phi(x)\rangle$ or $\langle\Phi^3(x)\rangle$ would lead to null terms in the vacuum. This becomes clear when we factorize the $\hat{\Phi}^2(x)$ terms in the Hamiltonian and blend them together so that

$$\hat{H} \to \hat{H}_{MF} = \frac{1}{2}\int dx\left[\hat{\Pi}^2(x) + [\nabla\hat{\Phi}]^2(x) + \left(m^2 + \frac{\lambda}{2}\langle\hat{\Phi}^2(x)\rangle\right)\hat{\Phi}^2(x)\right]. \tag{3.91}$$

In this expression the "new" mass is $m_*^2 = m^2 + \frac{\lambda}{2}\langle\hat{\Phi}^2(x)\rangle$. We shall restrict the mass to $m^2 > 0$ (the case $m^2 < 0$ shall be used in symmetry breaking models). We are actually doing an ansatz in the interacting theory, bringing it to a free theory form so that the interactions is thrown into the mass term. This effective mass is determined by the so called "gap equation"

$$\begin{aligned} m_*^2 &= m^2 + \frac{\lambda}{2}G(0) \\ &= m^2 + \frac{\lambda}{2}\int_{-\infty}^{+\infty}\frac{dp}{2\pi}\frac{1}{\sqrt{p^2+m_*^2}}\left[\frac{1}{e^{\beta\sqrt{p^2+m_*^2}}-1} + \frac{1}{2}\right], \end{aligned} \tag{3.92}$$

where we have used the $G(0)$ term from Eq. (3.83), but now with the new mass m_*^2. In order to solve this equation we need first to renormalized it because it is logarithmically divergent. This can be done by systematically using the appropriate counterterms in the model Hamiltonian. If one is interested only in the finite temperature contribution to m_*, one can subtract the zero temperature contribution at order λ and obtain [11]:

$$m_*^2 = m^2 + \frac{\lambda}{2}\int_{-\infty}^{+\infty}\frac{dp}{2\pi}\frac{1}{\sqrt{p^2+m_*^2}}\frac{1}{e^{\beta\sqrt{p^2+m_*^2}}-1}, \tag{3.93}$$

which is finite for any finite value of the temperature.

Chapter 4

Variational Method for Wigner Functionals

This chapter contains our original contribution to the Wigner functional theory in quantum field theory (QFT). We restrict our work to the $\lambda/4!\,\Phi^4$ theory in thermodynamical equilibrium, the theory discussed in the previous chapter. As mentioned in the Introduction, we transcribe to the QFT Wigner functional theory a variational method developed in statistical mechanics to go beyond the traditional mean field approximation for the free energy of nonrelativistic many-body theories. As mentioned in the Introduction, the method was first proposed in the context of the theory of superconductivity by Bogoliubov, Zubarev and Tserkovnikov (BZT) in Ref. [26] and further extended by Wentzel [28] to the theory of superfluidity. Later on, Girardeau [29] generalized the method to allow a wider range of applications.

The whole idea behind this variational method is to single out a number of possible scattering processes in the Hamiltonian of the theory to obtain a tractable problem using variational methods. One part of the full Hamiltonian, that contains only those selected processes, is quadratic in the fields and can be solved exactly, whereas the other part of the Hamiltonian is nonquadratic in the fields and should be treated in perturbation theory. Since the density matrix defining the free energy also defines the thermal Wigner functional, one can transcribe the formalism to the Wigner functional formalism to QFT in a straightforward manner. The method does not provide a criterion for choosing one or another process, the choice should be guided by the problem of interest. The traditional mean field approximation, in particular, refers to the direct and exchange scattering processes. In this work we abstract from any specific problem, and treat the method in its full generality.

We present in the beginning of the chapter a preview to the method, preparing the Hamiltonian of the model to obtain the density matrix to define the Wigner functional. Next, we obtain the gap equation that diagonalizes the quadratic

Hamiltonian. We show how the mean field approximation, discussed in the previous chapter, arises from the direct and exchange processes. We also compute the two point correlation function and the 2^{nd}-Rényi entropy corresponding to the quadratic Hamiltonian. We close the chapter with a numerical exercise.

4.1 The Variational Hamiltonian

In preparation for the application of the variational method to the Wigner functional formalism, we need to write the model Hamiltonian in momentum space. For simplicity of presentation and easy comparison with the results of Ref. [11], we write most of the formulas for the $1+1$ dimensional theory; the transcription to $d+1$ dimensions is straightforward, but we will make explicit those results that are valid for $d=1$ only. It is convenient to work with discrete momenta by quantizing the system in a box of volume $V = L$. As shown in Appendix B, by Fourier transforming the field $\hat{\Phi}(x)$ and conjugate momentum $\hat{\Pi}(x)$, the Hamiltonian in configuration space,

$$\hat{H} = \frac{1}{2}\int dx \left[\hat{\Pi}^2(x) + [\nabla\hat{\Phi}(x)]^2 + m^2\hat{\Phi}^2(x)\right] + \frac{\lambda}{4!}\int dx\, \hat{\Phi}^4(x)\,, \tag{4.1}$$

can be written in momentum space as:

$$\hat{H} = \hat{H}_0 + \hat{H}_I\,, \tag{4.2}$$

with

$$\hat{H}_0 = \frac{1}{2L}\sum_p \left[\hat{\Pi}^\dagger(p)\hat{\Pi}(p) + (\bar{p}^2 + m^2)\hat{\Phi}^\dagger(p)\hat{\Phi}(p)\right], \tag{4.3}$$

$$\hat{H}_I = \frac{\lambda}{4!}\frac{1}{L^3}\sum_{p,p',q} \hat{\Phi}^\dagger(p'+q)\hat{\Phi}^\dagger(p-q)\hat{\Phi}(p)\hat{\Phi}(p')\,. \tag{4.4}$$

where $\bar{p}$ in Eq. (4.3) indicates

$$\bar{p} = \begin{cases} \frac{2\pi}{L}n & \text{for } x \text{ continuous} \\ \frac{2}{a}\sin\left(\frac{\pi}{N}n\right) & \text{for } x \text{ discrete} \end{cases} \qquad \text{with } n = 0, \pm 1, \ldots\,. \tag{4.5}$$

In the latter case, $x \to x_l = la$, $l = 0, 1, \ldots, N-1$, where a is the lattice spacing and $L = Na$. In addition, the momentum indices vary as $n = -N/2+1, \ldots, 0, \ldots N/2$.

For the presentation of the formalism we do not need to specify which case we are using, but the numerical results we present at the end of this chapter are for the lattice discretization.

We show in Fig. 4.1 the convention for the momentum flow in the scattering processes implied by the Hamiltonian $\hat{H}_I$. At this stage, one can already identify special values of q, namely $q = 0$ and $q = p - p'$. They are special because they lead to a separable $\hat{H}_I$, that is, $\hat{H}_I$ can be written as the product of two terms of the form $\sum_p \hat{\Phi}^\dagger(p)\hat{\Phi}(p)$. Those q characterize *forward* and *exchange* processes, and lead to the mean field approximation discussed in the previous chapter. The variational Hamiltonian generalizes the mean field approximation implied by these two momenta and still leads to a tractable Wigner functional formalism.

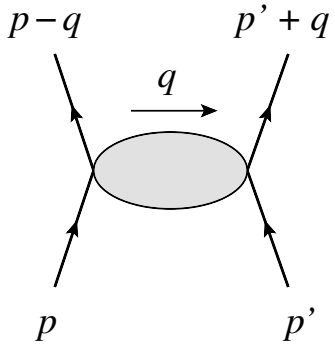

Figure 4.1: Momentum flow convention in a scattering process as implied by H_I in Eq. (4.4).

We start separating from the Hamiltonian $\hat{H}_I$ a set of transferred momenta q. Following Ref. [29], let $\mathcal{S}$ denote the set with the selected momenta $\mathcal{S}$ and $n(\mathcal{S})$ the corresponding density of states. For now, it is not necessary to specify $n(\mathcal{S})$, the only restriction is that $n(\mathcal{S})$ is independent of the volume in the thermodynamic limit. Therefore, we omit explicit reference to $n(\mathcal{S})$ in the following formulas. Specifically, we split $\hat{H}_I$ into two parts:

$$\hat{H}_I = \hat{H}_I(q \in \mathcal{S}) + \hat{H}_I(q \notin \mathcal{S})\,. \tag{4.6}$$

Next, we define operators $\hat{G}(q)$ and $\hat{G}(p,q)$ (in Ref. [29], $\hat{G}$ was denoted $\hat{\rho}$):

$$\hat{G}(q) = \frac{1}{L}\sum_p \hat{\Phi}^\dagger(p)\hat{\Phi}(p+q) = \frac{1}{L}\sum_p \hat{G}(p,q)\,, \tag{4.7}$$

so that one can rewrite $\hat{H}_I$ as

$$\begin{aligned}\hat{H}_I &= \frac{\lambda}{4!}\frac{1}{L}\sum_q \hat{G}^\dagger(q)\,\hat{G}(q) \\ &= \frac{\lambda}{4!}\frac{1}{L}\sum_{q\in\mathcal{S}} \hat{G}^\dagger(q)\hat{G}(q) + \frac{\lambda}{4!}\frac{1}{L}\sum_{q\notin\mathcal{S}} \hat{G}^\dagger(q)\,\hat{G}(q)\,. \end{aligned} \tag{4.8}$$

Finally, we rewrite $\hat{H}_I(q\in\mathcal{S})$ as

$$\begin{aligned}\hat{H}_I(q\in\mathcal{S}) &= \frac{\lambda}{4!}\frac{1}{L^3}\sum_p\sum_{p'}\sum_{q\in\mathcal{S}}\Big\{\Big[\hat{G}^\dagger(p,q)-g^*(p,q)\Big]\Big[\hat{G}(p',q)-g(p',q)\Big] \\ &\quad + g(p',q)\hat{G}^\dagger(p,q) + g^*(p,q)\hat{G}(p',q) - g^*(p,q)g(p',q)\Big\}\,. \end{aligned} \tag{4.9}$$

At this point, the functions $g(p,q)$ do not play any role, as they simply drop out. However, as we show in the following, they can be used as trial functions to define a variational Hamiltonian through the Gibbs variational principle applied to the full Hamiltonian. Having obtained the variational density matrix that gives the best approximation to the free energy, one can then use that density matrix to define the thermal Wigner functional.

The last term in Eq. (4.9) is independent of the fields; as such, we drop it from now on since it does not contribute in the computation of physical quantities. The full Hamiltonian can then be written as

$$\hat{H} = \hat{H}_q + \hat{H}'(q\in\mathcal{S}) + \hat{H}''(q\notin\mathcal{S}) \tag{4.10}$$

where we define $\hat{H}_q$ as being the Hamiltonian quadratic in the fields:

$$\begin{aligned}\hat{H}_q &= \frac{1}{2L}\sum_p\Big[\hat{\Pi}^\dagger(p)\hat{\Pi}(p) + (\bar{p}^2+m^2)\hat{\Phi}^\dagger(p)\hat{\Phi}(p)\Big] \\ &\quad + \frac{\lambda}{4!}\frac{1}{L^3}\sum_p\sum_{p'}\sum_{q\in\mathcal{S}}\Big[g(p',q)\hat{G}^\dagger(p,q) + g^*(p,q)\hat{G}(p',q)\Big]\,, \end{aligned} \tag{4.11}$$

and $\hat{H}'(q\in\mathcal{S})$ is nonquadratic in the fields:

$$\hat{H}'(q\in\mathcal{S}) = \frac{\lambda}{4!}\frac{1}{L^3}\sum_p\sum_{p'}\sum_{q\in\mathcal{S}}\Big[\hat{G}^\dagger(p,q)-g^*(p,q)\Big]\Big[\hat{G}(p',q)-g(p',q)\Big], \tag{4.12}$$

and $\hat{H}''(q \notin \mathcal{S}) = \hat{H}_I(q \notin \mathcal{S})$ is also nonquadratic:

$$\hat{H}''(q \notin \mathcal{S}) = \frac{\lambda}{4!}\frac{1}{L}\sum_{q \notin \mathcal{S}} \hat{G}^\dagger(q)\,\hat{G}(q)\,. \tag{4.13}$$

We show in the following how the Gibbs variational principle (GVP) can be used to obtain a gap equation for the functions $g(p,q)$ [29]. The GVP is reviewed in Appendix D; we reiterate here its relevant features for determining $g(p,q)$. Let $\hat{\rho}_\beta$ be the exact equilibrium density matrix corresponding to the full Hamiltonian of the model, Eq. (4.10):

$$\hat{\rho}_\beta = \frac{1}{Z}\,e^{-\beta\hat{H}}\,, \qquad Z = \mathrm{Tr}\,e^{-\beta\hat{H}}\,, \qquad \mathrm{Tr}\,\hat{\rho}_\beta = 1\,, \tag{4.14}$$

and $\hat{\rho}_\beta^{(q)}$ the equilibrium density matrix corresponding to $\hat{H}_q$:

$$\hat{\rho}_\beta^{(q)} = \frac{1}{Z^{(q)}}\,e^{-\beta\hat{H}_q}\,, \qquad Z^{(q)} = \mathrm{Tr}\,e^{-\beta\hat{H}_q}\,, \qquad \mathrm{Tr}\,\hat{\rho}_\beta^{(q)} = 1\,. \tag{4.15}$$

The GVP principle states that:

1. $\hat{\rho}_\beta$ minimizes the functional $\psi(\hat{\rho}) = \mathrm{Tr}\left(\hat{H}\hat{\rho}\right) + \frac{1}{\beta}\,\mathrm{Tr}\,(\hat{\rho}\ln\hat{\rho})$,
2. The Helmholtz free energy is given by $F = -\frac{1}{\beta}\ln Z = \psi(\hat{\rho}_\beta)$.

We have proven these results in Appendix D. We use these results to determine $g(p,q)$ as follows. First, we note that, since $\psi(\hat{\rho})$ computed with $\hat{\rho}_\beta$ is always smaller than when computed with any other density matrix, we have the inequality

$$F \leq \mathrm{Tr}\left(\hat{H}\,\hat{\rho}_\beta^{(q)}\right) + \frac{1}{\beta}\,\mathrm{Tr}\left(\hat{\rho}_\beta^{(q)}\ln\hat{\rho}_\beta^{(q)}\right) \equiv F_{var}(\hat{\rho}_\beta^{(q)})\,. \tag{4.16}$$

Second, the variational condition

$$\frac{\partial F_{var}(\hat{\rho}^{(q)})}{\partial g^*(p,q)} = 0\,, \tag{4.17}$$

is a necessary condition for a minimum of $F_{var}(\hat{\rho}^{(q)})$; this is a gap equation, a terminology borrowed from the theories of superconductivity and superfluidity.

Next, we derive explicit expression for the gap equation. Initially, we use $\hat{H} = \hat{H}_q + \hat{H}' + \hat{H}''$ in Eq. (4.16) to obtain

$$F_{var}(\hat{\rho}_\beta^{(q)}) = F_q + \langle H'\rangle_q + \langle H''\rangle_q\,, \tag{4.18}$$

where F_q is the Helmholtz free energy corresponding to $\hat{\rho}_\beta^{(q)}$:

$$F_q = -\frac{1}{\beta} \ln \mathrm{Tr}\; e^{-\beta \hat{H}_q} = -\frac{1}{\beta} \ln Z^{(q)} \,. \tag{4.19}$$

and the expectation values $\langle \cdots \rangle_q$ Eq. (4.18) are taken with respect to $\rho_\beta^{(q)}$:

$$\langle \cdots \rangle_q = \frac{1}{Z_\beta^{(q)}} \mathrm{Tr}\,(\cdots) e^{-\beta \hat{H}_q} \,. \tag{4.20}$$

Now, one can show [29] that, in the thermodynamic limit, the variational condition in Eq. (4.17) is satisfied by

$$\begin{aligned} g(p,q) &= \langle \hat{G}(p,q) \rangle_q = \langle \hat{\Phi}^\dagger(p) \hat{\Phi}(p+q) \rangle_q \\ &= \frac{1}{Z_\beta^{(q)}} \mathrm{Tr} \left[\hat{\Phi}^\dagger(p) \hat{\Phi}(p+q) e^{-\beta \hat{H}_q} \right] . \end{aligned} \tag{4.21}$$

The proof of this result is outlined in Ref. [29] using Hilbert space methods. In particular, Ref. [29] proves that $\langle H' \rangle_q = 0$ and $\langle H'' \rangle_q = 0$ if Eq. (4.21) is satisfied. We do not repeat that proof here, as a step by step demonstration can be found in Ref. [30]. But for completeness, we use the Wigner functional formalism to prove that $\langle H' \rangle_q = 0$ and $\langle H'' \rangle_q = 0$.

Equation (4.21) is a nonlinear equation for the functions $g(p,q)$, as $\hat{H}_q$ depends on the $g(p,q)$. To obtain an explicit expression for this nonlinear equation, it is convenient to have $\hat{H}_q$ in diagonal form in the field operators, because then one can compute the expectation value $\langle \hat{\Phi}^\dagger(p) \hat{\Phi}(p+q) \rangle_q$ in closed form. In the next section we discuss the diagonalization of $\hat{H}_q$.

4.2 Diagonalization of $\hat{H}_q$

The Hamiltonian $\hat{H}_q$ is quadratic in $\hat{\Phi}$ and $\hat{\Pi}$. It is diagonal in Π but not in Φ. To obtain an explicit expression for the gap equation determining the $g(p,q)$ trial functions, we need to diagonalize $\hat{H}_q$. As we will show in Section 4.4, the gap equation we obtain is similar to Eq. (3.92) for the effective mass m_* in the mean field approximation. In fact, we recover Eq. (3.92) by restricting the scattering processes to the direct and exchange processes, characterized by the momenta $q = 0$ and $q = p - p'$, shown in Fig. 4.2.

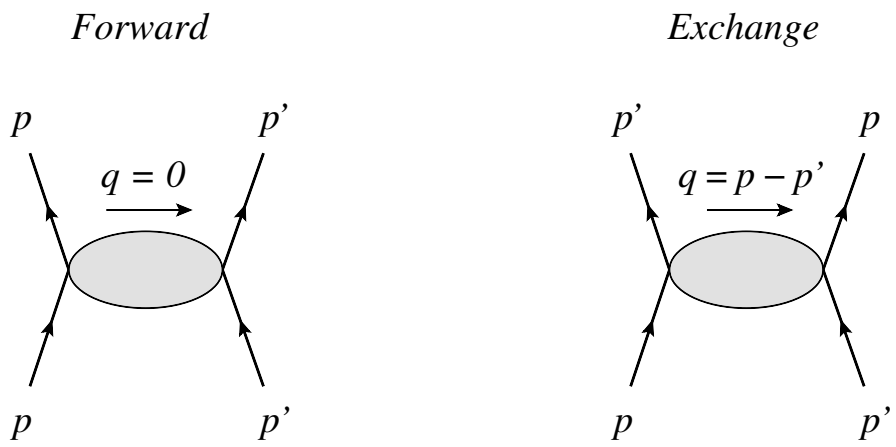

Figure 4.2: Scattering processes in H_I leading to the mean field approximation.

We start rewriting $\hat{H}_q$ given in Eq. (4.11) as

$$\hat{H}_q = \hat{H}_q(\Pi, \Phi) = \hat{H}_q(\Pi) + \hat{H}_q(\Phi)\,, \tag{4.22}$$

with

$$\hat{H}_q(\Pi) = \frac{1}{2L}\sum_p \hat{\Pi}^\dagger(p)\hat{\Pi}(p)\,, \tag{4.23}$$

$$\hat{H}_q(\Phi) = \frac{1}{2L}\sum_{p,p'} \mathcal{E}^2(p,p')\,\hat{\Phi}^\dagger(p)\hat{\Phi}(p')\,, \tag{4.24}$$

with $\mathcal{E}^2(p,p')$ being the energy matrix:

$$\begin{aligned}\mathcal{E}^2(p,p') &= \mathcal{E}^2_D(p)\,\delta_{pp'} \\ &\quad + 2\,\frac{1}{L^2}\frac{\lambda}{4!}\sum_{q\in\mathcal{S}}{}' \left[\delta_{p',p+q}\sum_{p''} g^*(p'',q) + \delta_{p',p-q}\sum_{p''} g(p'',q)\right],\end{aligned} \tag{4.25}$$

where the diagonal part $\mathcal{E}^2_D(p)$ is given by

$$\mathcal{E}^2_D(p) = \bar{p}^2 + m^2 + 3\times 2\,\frac{1}{L^2}\frac{\lambda}{4!}\sum_{p'}\left[g^*(p',0) + g(p',0)\right]\,. \tag{4.26}$$

The factor 3 comes from the contributions with $q = 0$, $q = p - p' > 0$, and $q = p - p' < 0$, and the $'$ in $\sum'_q$ in Eq. (4.25) indicates that the sum does not contain these q values. This shows that the direct and exchange contributions are equal, which is a feature of the contact-interaction nature of the Φ^4 interaction; for

finite-range interactions, this is not the case [29].

Before we proceed, we recall that we have omitted in the above explicit reference to the density of states $n(\mathcal{S})$. This is crucial element in the method, as $n(\mathcal{S})$ determines the weight with which the different scattering processes contribute to the energy matrix $\mathcal{E}^2(p,p')$. We come back to this issue in Section 4.4. It is also important to make clear the meaning of the delta functions $\delta_{p,p+q}$ and $\delta_{p,p'+q}$ in Eq. (4.25). These delta functions reflect the fact that for generic values of q, the single-particles energies $\mathcal{E}^2(p,p')$ are nondiagonal, reflecting off-diagonal transitions induced by single-particle $p \to p'$ rescattering processes. The energy being nondiagonal signals that different momentum modes are entangled, i.e. different momentum modes are not independent from each other. Since different momentum modes are entangled, one cannot write the energy as a sum of the energies of each mode. Also, the density matrix in the basis of the field operators $\hat{\Phi}$ is not a product of density matrices for each momentum mode. Now for the special values of q discussed above, the final state momenta in the scattering contributing to $\mathcal{E}^2(p,p')$ are the same of the initial state, as depicted by the two graphs in Fig. 4.2. In these very special cases, $\mathcal{E}^2(p,p')$ is diagonal, reflecting $p \to p$ rescattering processes. In addition, one one can write the energy as sum of the energies of each mode, and the corresponding density matrix is a product state in the basis of the field Φ .

The Hamiltonian $\hat{H}_q$ can be diagonalized by a linear canonical transformation on the field operators $\hat{\Phi}^\dagger(p)$ and $\hat{\Phi}(p)$:

$$\hat{\Phi}(p) = \sum_{p'} U(p,p')\,\hat{\chi}(p')\,, \tag{4.27}$$

where $U(p,p')$ is a unitary matrix, which connects momenta p and $p+q$ with $q \in \mathcal{S}$. Since the unitary transformation is time independent and $\hat{\Pi} = -i\frac{\delta}{\delta\hat{\Phi}}$, one can write

$$\hat{\Pi}(p) = \sum_{p'} U(p,p')\,\hat{\Pi}_\chi(p')\,. \tag{4.28}$$

Unitarity of U means:

$$UU^\dagger = U^\dagger U = 1 \to \sum_k U(p,k)U^*(p',k) = \sum_k U^*(k,p)U(k,p') = \delta_{pp'}. \tag{4.29}$$

We then apply this transformation to the $\hat{\Pi}$- and $\hat{\Phi}$-dependent terms in Eqs. (4.23)

and (4.24). The $\hat{\Pi}$-dependent terms transforms trivially:

$$\begin{aligned}\sum_p \hat{\Pi}^\dagger(p)\hat{\Pi}(p) &= \sum_{p,p',p''} U^*(p',p)\Pi^\dagger_\chi(p')U(p,p'')\hat{\Pi}_\chi(p'') \\ &= \sum_p \hat{\Pi}^\dagger_\chi(p)\hat{\Pi}_\chi(p)\,, \end{aligned} \tag{4.30}$$

whereas the $\hat{\Phi}$-dependent term transforms nontrivially:

$$\hat{H}_q(\Phi) = \frac{1}{2L}\sum_p\sum_{p'}\sum_k\sum_{k'} U^*(k,p)\,\mathcal{E}^2(p,p')\,U(p',k')\hat{\chi}^\dagger(k)\,\hat{\chi}(k'). \tag{4.31}$$

If we denote $\phi_k(p)$ the orthonormalized eigenvectors of $\mathcal{E}^2(p,p')$ and $\omega^2(k)$ the corresponding eigenvalues:

$$\sum_{p'} \mathcal{E}^2(p,p')\,\phi_k(p') = \omega^2(k)\,\phi_k(p)\,, \tag{4.32}$$

and take

$$U(p,k) = \phi_k(p)\,, \tag{4.33}$$

one obtains $\hat{H}_q[\Phi]$ in diagonal form, namely:

$$\hat{H}_q(\Phi) \to \hat{H}_q(\chi) = \frac{1}{2L}\sum_p \omega^2(p)\,\hat{\chi}^\dagger(p)\hat{\chi}(p)\,. \tag{4.34}$$

The complete $\hat{H}_q$ is then in diagonal form:

$$\hat{H}_q(\Pi,\Phi) \to \hat{H}_q(\Pi_\chi,\chi) = \frac{1}{2L}\sum_p \left[\hat{\Pi}^\dagger_\chi(p)\hat{\Pi}_\chi(p) + \omega^2(p)\,\hat{\chi}^\dagger(p)\hat{\chi}(p)\right]. \tag{4.35}$$

In terms of continuum momenta, $\hat{H}_q(\Pi_\chi,\chi)$ is given by:

$$\begin{aligned}\hat{H}_q(\Pi_\chi,\chi) &= \frac{1}{2}\int_{-\infty}^{\infty}\frac{dp}{2\pi}\left[\hat{\Pi}^\dagger_\chi(p)\hat{\Pi}_\chi(p) + \omega^2(p)\,\hat{\chi}^\dagger(p)\hat{\chi}(p)\right] \\ &= \int_0^{\infty}\frac{dp}{2\pi}\left[\hat{\Pi}^\dagger_\chi(p)\hat{\Pi}_\chi(p) + \omega^2(p)\,\hat{\chi}^\dagger(p)\hat{\chi}(p)\right]. \end{aligned} \tag{4.36}$$

4.3 The Wigner Functional from $\hat{H}_q$

To obtain the gap equation, we need to have an explicit expression for the expectation value $\left\langle \hat{\Phi}^\dagger(p)\hat{\Phi}(p+q)\right\rangle_q$. Therefore, we need to be able to compute, more generally, expectation values of operators $\hat{\mathcal{O}}(\hat{\Pi},\hat{\Phi})$ using the Wigner functional corresponding to $\hat{H}_q$. To do so, we use the density matrix given in Eq. (4.15), expressing $\hat{H}_q$ in terms of the $\hat{\Pi}_\chi(p)$ and $\hat{\chi}(p)$ field operators. We do this because $\hat{H}_q$ is diagonal in those fields and one can follow the same derivation steps used in the calculations of the Wigner functional for $\hat{H}_0$ (which is diagonal in the fields $\hat{\Pi}$ and $\hat{\Phi}$). Since the Jacobian of the transformation from the $\hat{\Phi}$ to $\hat{\chi}$ fields is unity, one can take over the result in Eq. (3.65) and write:

$$\begin{aligned} W_\beta^{(q)}(\chi,\Pi_\chi) &= \int D\varphi(p)\, e^{-i\int_{-\infty}^{\infty} dx\,\Pi_\chi(p)\varphi(p)} \left\langle \chi(p)+\frac{\varphi(p)}{2}\,\middle|\,\hat{\rho}(t)\,\middle|\,\chi(p)-\frac{\varphi(p)}{2}\right\rangle \\ &= C_\beta^{(q)}\, e^{-\frac{\beta}{2}\int_{-\infty}^{\infty}\frac{dp}{2\pi}\tilde{\Delta}_\beta^\omega(p)\left[\Pi_\chi^*\Pi_\chi+\omega^2(p)\chi^*(p)\chi(p)\right]} \end{aligned} \tag{4.37}$$

in which the thermal weight factor $\tilde{\Delta}_\beta^\omega(p)$ is now given by

$$\tilde{\Delta}_\beta^\omega(p) = \frac{2}{\beta\omega(p)}\tanh\frac{\beta\omega(p)}{2}\,, \tag{4.38}$$

and the normalization C^ω by

$$C_\beta^{(q)} = \exp\left[L\int_{-\infty}^{\infty}\frac{dp}{2\pi}\ln\left(2\tanh\frac{\beta\omega(p)}{2}\right)\right]\,. \tag{4.39}$$

To compute $\hat{\mathcal{O}}(\hat{\Pi},\hat{\Phi})$ using this Wigner functional, we rewrite $\hat{\mathcal{O}}(\hat{\Pi},\hat{\Phi})$ in terms of the $\hat{\Pi}_\chi$ and $\hat{\chi}$:

$$\hat{\mathcal{O}}(\hat{\Pi},\hat{\Phi}) = \hat{\mathcal{O}}(U\hat{\Pi}_\chi, U\hat{\chi})\,. \tag{4.40}$$

Then, one can write

$$\left\langle\hat{\mathcal{O}}(\hat{\Pi},\hat{\Phi})\right\rangle_q = \left\langle\hat{\mathcal{O}}(U\hat{\Pi}_\chi,U\hat{\chi})\right\rangle_q = \mathrm{Tr}\left[\hat{\mathcal{O}}(U\hat{\Pi}_\chi,U\hat{\chi})\,\hat{\rho}_\beta^{(q)}\right], \tag{4.41}$$

with $\hat{\rho}_\beta^{(q)}$ being the equilibrium density matrix given in Eq. (4.15). Computing the

traces in the basis of the eigenstates of the $\hat{\chi}$ and $\hat{\Pi}_\chi$ field operators:

$$\begin{aligned} \hat{\chi}(p)\,|\chi(p)\rangle &= \chi(p)\,|\chi(p)\rangle\,, \\ \hat{\Pi}_\chi(p)\,|\Pi_\chi(p)\rangle &= \Pi_\chi(p)\,|\Pi_\chi(p)\rangle\,, \end{aligned} \tag{4.42}$$

we can now follow the derivation for $\hat{H}_0$. Again, due to the unitarity of U, the integration measure is invariant under the $\hat{\Phi}$ to $\hat{\chi}$ transformation, and one can write:

$$\begin{aligned} \left\langle \hat{\mathcal{O}}(\hat{\Pi},\hat{\Phi})\right\rangle_q &= \mathrm{Tr}\left[\hat{\mathcal{O}}(U\hat{\Pi}_\chi, U\hat{\chi})\,\hat{\rho}_\beta^{(q)}\right] \\ &= \int D\chi \frac{D\Pi_\chi}{2\pi}\,\mathcal{O}(U\hat{\Pi}_\chi, U\hat{\chi})\,W_\beta^{(q)}(\chi,\Pi_\chi)\,. \end{aligned} \tag{4.43}$$

In the following, we will need $\left\langle \hat{\Phi}^\dagger(p)\hat{\Phi}(p)\right\rangle_q$. This can be computed using the result just derived, Eq. (4.43), namely:

$$\begin{aligned} \left\langle \hat{\Phi}^\dagger(p)\hat{\Phi}(p)\right\rangle_q &= \int D\Phi \frac{D\Pi}{2\pi}\,\Phi^\dagger(p)\Phi(p)\,W_\beta^{(q)}(\Phi,\Pi) \\ &= \sum_{k,k'} U^*(p,k)U(p,k') \int D\chi \frac{D\Pi_\chi}{2\pi}\,\chi^*(k)\chi(k')\,W_\beta^{(q)}(\chi,\Pi_\chi) \\ &= \sum_{k} U^*(p,k)U(p,k) \int D\chi \frac{D\Pi_\chi}{2\pi}\,\chi^*(k)\chi(k)\,W_\beta^{(q)}(\chi,\Pi_\chi), \end{aligned} \tag{4.44}$$

where in the last step we used the fact that the functional integral is different from zero only for $k = k'$, as can be verified very easily using the methods in Appendix C. Now, we simply transcribe the result obtained previously for $\left\langle \hat{\Phi}^\dagger(k)\,\hat{\Phi}(k)\right\rangle_0$ in Eq. (3.72):

$$\begin{aligned} \left\langle \hat{\Phi}^\dagger(p)\hat{\Phi}(p)\right\rangle_q &= L\sum_k \frac{U^*(p,k)\,U(p,k)}{\beta\,\tilde{\Delta}_\beta(k)\omega^2(k)} \\ &= L\sum_k \frac{1}{\omega(k)}\frac{U^*(p,k)\,U(p,k)}{e^{\beta\omega(k)}-1} + \frac{L}{2}\sum_k \frac{U^*(p,k)\,U(p,k)}{\omega(k)} \\ &= L\sum_k \frac{1}{\omega(k)}\phi_k^*(p)\,\phi_k(p)\left(\frac{1}{e^{\beta\omega(k)}-1}+\frac{1}{2}\right), \end{aligned} \tag{4.45}$$

where we replaced $U(p,k)$ by $\phi_k(p)$; see Eq. (4.33). When $\phi_k(p) = \delta_{kp}$, i.e. when the energy matrix $\mathcal{E}^2(p,p')$ is diagonal in the fields Φ, Eq. (4.45) collapses to the

result obtained in the previous chapter, namely Eq. (3.72).

Another quantity of interest we can compute with $W_\beta^{(q)}[\Phi,\Pi]$ is the equivalent to the quantum mechanical 2−Rényi entropy S_2, defined in Eq. (3.44). Specifically, the S_2 corresponding to $W_\beta^{(q)}[\Phi,\Pi]$, which we denote $S_2^{(q)}$, is given by

$$S_2^{(q)} = -\ln \mathrm{Tr}\left(\hat{\rho}_\beta^{(q)}\right)^2 = -\ln \int D\Phi \frac{D\Pi}{2\pi}\left(W_\beta^{(q)}[\Phi,\Pi]\right)^2 . \tag{4.46}$$

We note that it is important to work with a properly normalized $\hat{\rho}_\beta^{(q)}$, as in Eq. (4.15). Repeating the computations in Appendix C.3 by taking into account the explicit appearance of the partition function in $\hat{\rho}_\beta^{(q)}$, we obtain for the functional integral of $\left(W_\beta^{(q)}[\Phi,\Pi]\right)^2$ the following result:

$$\begin{aligned}\int D\Phi \frac{D\Pi}{2\pi}\left(W_\beta^{(q)}[\Phi,\Pi]\right)^2 &= \left(C_\beta^{(q)}\right)^2 \exp\left[L\int_{-\infty}^{\infty}\frac{dp}{2\pi}\ln\left(4\tanh\frac{\beta\omega(p)}{2}\right)\right] \\ &= \exp\left\{L\int_{-\infty}^{\infty}\frac{dp}{2\pi}\left[2\ln\left(2\tanh\frac{\beta\omega(p)}{2}\right)-\ln\left(4\tanh\frac{\beta\omega(p)}{2}\right)\right]\right\} \\ &= \exp\left[L\int_{-\infty}^{\infty}\frac{dp}{2\pi}\ln\left(\tanh\frac{\beta\omega(p)}{2}\right)\right] .\end{aligned} \tag{4.47}$$

After taking the ln of this result, one obtains for 2-Rényi entropy $S_2^{(q)}$:

$$S_2^{(q)} = -L\int_{-\infty}^{\infty}\frac{dp}{2\pi}\ln\left(\tanh\frac{\beta\omega(p)}{2}\right) . \tag{4.48}$$

In the zero temperature limit ($\beta\to\infty$) we obtain a vanishing entropy. This is the correct result since at zero temperature we are dealing with the vacuum state, which is a pure state. When the state is pure, one has the maximum possible information about the system.

4.4 The Gap Equation

With the result of Eq. (4.45), the gap equation becomes

$$\begin{aligned} g(p,q) &= \left\langle \hat{\Phi}^{\dagger}(p)\hat{\Phi}(p+q)\right\rangle_q \\ &= \sum_{k,k'} U^*(p,k)U(p+q,k') \int D\chi \frac{D\Pi_\chi}{2\pi}\, \chi^*(k)\chi(k')\, W_\beta^{(q)}(\chi,\Pi_\chi) \\ &= \sum_{k} U^*(p,k)U(p+q,k) \int D\chi \frac{D\Pi_\chi}{2\pi}\, \chi^*(k)\chi(k)\, W_\beta^{(q)}(\chi,\Pi_\chi) \\ &= \sum_{k} \phi_k^*(p)\,\phi_k(p+q)\,\frac{L}{\omega(k)}\left(\frac{1}{e^{\beta\omega(k)}-1}+\frac{1}{2}\right), \end{aligned} \tag{4.49}$$

where again we replaced $U(p,k)$ by $\phi_k(p)$. Equation (4.49) is a nonlinear equation, as the right hand side is a functional of $g(p,q)$ through $\omega(k)$ and $\phi_k(p)$. Moreover, we need to specify the qs and corresponding weights $n(\mathcal{S})$.

What processes does one need to use? As mentioned at the beginning of this chapter, the answer to this question depends on the physics of the problem at hand. For example, the physics of the problem might be driven by scattering processes defined by a few values of transferred momenta. Classical examples include those for which the direct and exchange scattering processes suffice to describe the main features of the phenomena one wants to describe. In that case, all the weight $n(\mathcal{S})$ would be on those processes. But for other systems, it might happen that those direct and exchange contributions are no more, or even are less important than others that lead to off-diagonal contributions to the energy $\mathcal{E}^2(p,p')$.

Although the model we are using, a real scalar field in $1+1$ spacetime dimensions, is adequate for our purposes of presenting the use of the variational method in the Wigner functional formalism, unfortunately it is not rich enough for phenomenologically interesting applications. Besides the inherent limitations of one-dimensional scattering, a real scalar field cannot describe phenomena like superfluidity, condensate formation and phase transition phenomena. But the structure of the energy matrix $\mathcal{E}^2(p,p')$ reveals a feature that one will face when tackling more realistic models regarding the role played by the weight $n(\mathcal{S})$. There is a relatively large imbalance in the contributions of the interaction in favor of the diagonal elements of the matrix, namely: a diagonal element comes multiplied by 12 whereas a off-diagonal term comes multiplied by 2. Therefore, if the

diagonal and off-diagonal terms enter with equal weight, in the sense that $n(\mathcal{S})$ is taken as process independent, the off-diagonal terms are, from the outset, one order of magnitude smaller than the diagonal ones. Moreover, the off-diagonal overlaps $\phi_k^*(p)\phi_k(p+q)$, that enter the gap equation in Eq. (4.4), will then be small, magnifying the smallness of the off-diagonal elements of $\mathcal{E}^2(p,p')$.

In view of the limitations of the model, we will examine the consequences of decreasing the weight with which the direct and exchange processes contribute to $\mathcal{E}^2(p,p')$ while increasing the weight of the off-diagonal contributions. The exact way we change the weight is explained shortly ahead when we discuss numerical results. It should be clear that this is a theoretical exercise with the sole aim of illustrating the effect of the off-diagonal elements of $\mathcal{E}^2(p,p')$ on the spectrum, correlation function, and entropy. It is also worth mentioning that we are unaware of any other study in the literature with which we could compare results.

The contributions of the direct and exchange processes, shown in Fig. 4.2, lead to a diagonal energy $\mathcal{E}(p,p')$ matrix with elements $E_D(p)$. The eigenvalues $\omega_*^2(p)$ are of course the diagonal elements of the matrix:

$$\omega_*^2(p) = E_D(p) = \bar{p}^2 + m_*^2\,, \tag{4.50}$$

where

$$m_*^2 = m^2 + 6\,\frac{\lambda}{4!}\,\frac{1}{L^2}\sum_p \left[g^*(p,0) + g(p,0)\right]. \tag{4.51}$$

Using the gap equation, Eq. (4.49), for $g(p,0)$ into Eq. (4.51), one obtains for m_*^2:

$$\begin{aligned} m_*^2 &= m^2 + 6\,\frac{\lambda}{4!}\,\frac{1}{L^2}\sum_k \frac{L}{\omega_*(k)}\left[\frac{1}{e^{\beta\omega_*(k)}-1}+\frac{1}{2}\right]\,2\sum_p U^*(p,k)\,U(p,k) \\ &= m^2 + \frac{\lambda}{2}\,\frac{1}{L}\sum_k \frac{1}{\omega_*(k)}\left(\frac{1}{e^{\beta\omega_*(k)}-1}+\frac{1}{2}\right) \\ &\to m^2 + \frac{\lambda}{2}\int_{-\infty}^{\infty}\frac{dk}{2\pi}\,\frac{1}{\omega_*(k)}\left(\frac{1}{e^{\beta\omega_*(k)}-1}+\frac{1}{2}\right). \end{aligned} \tag{4.52}$$

which is the mean field result given in Eq. (3.92). This equation can be solved numerically on a lattice.

Now, when other than the direct and exchange processes are taken into account, to obtain the Wigner functional $W_\beta^{(q)}[\Phi,\Pi]$, Eq. (4.37), we need to compute the

eigenvalues $\omega^2(k)$ and corresponding eigenfunctions $\phi_k(p)$ of the matrix $\mathcal{E}^2(p,p')$. As mentioned earlier, we are dealing with a nonlinear problem, in that to determine $\omega^2(k)$ and $\phi_k(p)$, we need the $g(p,q)$ to obtain $\mathcal{E}^2(p,p')$, but the functions $g(p,q)$ depend on $\omega^2(k)$ and $\phi_k(p)$. We approach the solution of this nonlinear problem by an iterative scheme. We explain how precisely we do this in Section 4.6. We present illustrative numerical results in Section 4.6.

We still have the contributions of H' and H''. We discuss them in the next section. H' and H'' are required, e.g. to explore features associated with the negativity of the Wigner functional. This is because $W_\beta^{(q)}$ is a single Gaussian. Of course, this $W_\beta^{(q)}$ does describe entanglement of the Φ field momentum modes that the mean field approximation misses.

4.5 The Terms $\hat{H}'$ and $\hat{H}''$

Up to now, we have addressed the problem of diagonalizing $\hat{H}_q$ to obtain the gap functions $g(p,q)$. These gap functions enter explicitly in $\hat{H}'$ and implicitly in $\hat{H}''$ through the selection of $\mathcal{S}$. As already mentioned, the contributions of $\hat{H}'$ and $\hat{H}''$ to physical quantities should be computed in perturbation theory. The relative importance of their contributions depends crucially on how much of the physics of the problem at hand is captured by $\hat{H}_q$. But if one knows the Wigner functional $W_\beta^{(q)}[\Phi,\Pi]$, one can compute the contributions of $\hat{H}'$ and $\hat{H}''$ in a straightforward manner.

A key quantity in the computation of thermodynamical quantities is the partition function Z_β. It is a feature of the method that $\hat{H}'$ does not contribute to Z_β in all orders of perturbation theory, whereas $\hat{H}''$ only contributes to Z_β at second and higher orders. These features were proved in Ref. [29] using traditional Hilbert space methods. In the following, we outline a proof, using mixed Hilbert space and Wigner functional techniques, that the first order contributions of $\hat{H}'$ and $\hat{H}''$ vanish. Although this is a somewhat trivial exercise, it nevertheless serves the purpose of illustrating the way one would compute perturbative corrections to the Wigner functional itself using Hilbert space techniques in the context of the Wigner functional formalism. We come back to this shortly ahead.

We start from the definition of the partition function:

$$Z = \mathrm{Tr}\, e^{-\beta(\hat{H}_q+\hat{H}'+\hat{H}'')}\,. \tag{4.53}$$

We use the well known expression:

$$e^{-\beta(\hat{H}_q+\hat{H}'+\hat{H}'')} = e^{-\beta\hat{H}_q}\left[1-\int_0^\beta d\tau\, e^{\tau\hat{H}_q}\left(\hat{H}'+\hat{H}''\right)\, e^{-\tau\hat{H}_q}+\cdots\right], \tag{4.54}$$

so that

$$Z_\beta = \mathrm{Tr}\, e^{-\beta(\hat{H}_q+\hat{H}'+\hat{H}'')} = Z_\beta^{(q)} + Z_\beta^{(1)} + \cdots, \tag{4.55}$$

where $Z_\beta^{(q)}$ is the partition function corresponding to $\hat{H}_q$ and

$$Z_\beta^{(1)} = \int_0^\beta d\tau\ \mathrm{Tr}\left[e^{-\beta\hat{H}_q}\, e^{\tau\hat{H}_q}\left(\hat{H}'+\hat{H}''\right)\, e^{-\tau\hat{H}_q}\right]. \tag{4.56}$$

Using the cyclic property of the trace, we can write $Z^{(1)}$ as

$$\begin{aligned} Z_\beta^{(1)} &= -\int_0^\beta d\tau\ \mathrm{Tr}\left[e^{-\beta\hat{H}_q}\, e^{\tau\hat{H}_q}\left(\hat{H}'+\hat{H}''\right)\, e^{-\tau\hat{H}_q}\right] \\ &= -\beta\,\mathrm{Tr}\left[e^{-\beta\hat{H}_q}\,\left(\hat{H}'+\hat{H}''\right)\right] = Z_\beta^{(q)}\,\left[-\beta\left\langle\hat{H}'+\hat{H}''\right\rangle_q\right]. \end{aligned} \tag{4.57}$$

Therefore, using the results proven earlier regarding computation of expectation values with the Wigner functional, we can write

$$Z^{(1)} = -\beta\, Z_\beta^{(q)} \int D\Phi\, \frac{D\Pi}{2\pi}\, W_\beta^{(q)}[\Phi,\Pi]\,\left(\hat{H}'[\Phi]+\hat{H}''[\Phi]\right). \tag{4.58}$$

We consider first $\left\langle\hat{H}'\right\rangle_q$. Inserting the expression in Eq. (4.12) for $\hat{H}'$ and using the fact that it depends on Φ only, we can write

$$\begin{aligned} \left\langle\hat{H}'\right\rangle_q = \frac{\lambda}{4!}\frac{1}{L^3}\sum_{p,p'}\sum_{q\in\mathcal{S}}\int D\Phi\, W_\beta^{(q)}[\Phi]\,\Big[&G^*(p,q)G(p',q) - g(p',q)G^*(p,q) \\ &- g^*(p,q)G(p',q) + g^*(p,q)g(p',q)\Big]. \end{aligned} \tag{4.59}$$

Next, we change from Φ to χ, and use the gap equation for the $g(p',q)G^*(p,q)$ and $g^*(p,q)G(p',q)$. This leads to the cancellation between these terms and $g^*(p,q)g(p',q)$, with the net result $-g^*(p,q)g(p',q)$. We are then left with an integral involving four χ fields:

$$\int D\chi\, W_\beta^{(q)}[\chi]\,\chi^*(k_4)\,\chi^*(k_3)\,\chi(k_2)\,\chi(k_1). \tag{4.60}$$

Since $W_\beta^{(q)}[\chi]$ is quadratic and diagonal in $\chi(k)$, one can easily show, using the methods of Appendix C, that this integral factorizes into products of two integrals of a pair of fields $\chi^*(k)\chi(k')$. This is nothing else then Wick's theorem at work in the context of the Wigner functional formalism. Using again the gap equation for each of such integrals, and working out the combinatoric factors coming from the different pairings among the $k_1, \cdots, k_4$, one obtains that the integrals cancel the term $g^*(p,q)g(p',q)$, and one establishes the result that $\langle \hat{H}' \rangle_q$ vanishes.

Now, the proof that $\langle \hat{H}'' \rangle_q$ vanishes is trivial. The unitary transformation $U(p,p')$ connects momenta p and $p' = p \pm q$ with $q \in \mathcal{S}$—see Eq. (4.25). But $\hat{H}''$ excludes $q \in \mathcal{S}$, as such, Eq. (4.60) is zero trivially in this case.

The contributions of $\hat{H}'$ and $\hat{H}''$ to the full Wigner functional itself should be computed in perturbation theory as well. It is out of the scope of this work to compute such contributions, but we must stress that they are an important aspect to the variational method. They are important because they provide a self-consistency check on a specific application, in that their contributions should provide "corrections" to the zeroth-order results computed with $\hat{H}_q$. That is, if $\hat{H}_q$ does capture most of the physics of the problem, then the remaining parts of the full Hamiltonian should not have a large impact on the results. Moreover, it is conceivable that $\hat{H}_q$ describes well some observables, like bulk thermodynamical properties of the system, but it does not describe well more subtle properties, like e.g. those for which the entanglement of momentum modes is the dominant effect. In such a situation, one needs to compute those perturbative corrections.

There exist well-advanced techniques to compute perturbative corrections to the Wigner function both in quantum mechanics [58, 12, 59] and quantum field theory [16], without the use of Hilbert space techniques as we used in the demonstration above. One difficulty one faces to implement perturbation theory directly to the the Wigner function is the appearance of off-diagonal generalized Wigner functions, originally introduced by Moyal in Ref. [47], which are technically involved. In this respect, techniques based on generating functionals as those of Ref. [16] lead to compact evaluations.

4.6 Numerical Results

We solved numerically the nonlinear eigenvalue problem using lattice discretization. We followed the procedure of Monte Carlo lattice simulations of quantum field theories, in that we rescaled all dimensionful quantities by the

lattice spacing a so that the lattice spacing does not appear in the equations. At the end of the simulations, one can restore the physical dimensions of computed observables to fix the lattice spacing by a procedure known as scale setting and renormalization. The scalar theory in $1+1$-dimensions is superrenomalizable, i.e. there is only one divergent Feynman diagram, the one-loop tadpole. Such a divergence is reflected by the factor $1/2$ in, e.g., Eqs. (4.45) and (4.49). We followed Ref. [11] to simplify this procedure: we consider only the finite temperature contribution, which means that we eliminated the factor $1/2$ in Eqs. (4.45) and (4.49) by subtracting the corresponding zero temperature contribution, as explained previously. In principle, we would still need to take the $N \to \infty$ limit; in lattice simulations of quantum field theories, this limit is usually taken by using finite size scaling theory. In this work we did not take the $N \to \infty$ limit, we simply checked the stability of the results by changing N.

For the $1+1$ scalar field theory, the mass dimension of the relevant quantities are (recall we are using $\hbar = c = 1$):

$$[\Phi(p)] = -1, \quad [\Pi(p)] = 0, \quad [m] = 1, \quad [\lambda] = 2, \quad [\beta] = -1\,. \tag{4.61}$$

Here and in the following, we denote with a hat $\hat{}$ the dimensionless rescaled quantities. The appropriate rescalling of the dimensionful quantities are :

$$m = a^{-1}\,\hat{m}, \quad \lambda = a^{-2}\,\hat{\lambda}, \quad \Phi(p) = a\,\hat{\Phi}(p), \quad \beta = a\,\hat{\beta}\,. \tag{4.62}$$

We present results in terms of the dimensionless quantities, so that we do not need to specify the energy scale through the lattice spacing.

We made the numerical calculations using a code written in the Python language. We used the intrinsic `scipy.linalg` package to obtain the eigenvalues and eigenvectors. As mentioned in Section 4.4, we solved the problem by iteration. Our iteration procedure was essentially the one proposed in Ref. [29], namely:

1. We started the iteration with simple ansätze for $\omega^2(k)$ and $\phi_k(p)$, we used the noniteracting single-particle energy, $\omega^2(k) = \bar{p}^2 + m^2$, and took $\phi_k(p) = (1, 1, \cdots, 1)/\sqrt{N}$, where N is the number of lattice sites;

2. We then computed the $g(p,q)$ with these ansätze and determined the energy matrix $\mathcal{E}^2(p,p')$;

3. Then we computed the eigenvalues $\omega^2(k)$ and eigenfunctions $\phi_k(p)$ of $\mathcal{E}^2(p,p')$ obtained in 2);

4. With the $\omega(k)$ and $\phi_k(p)$ found in 3), we computed again $g(p,q)$ and $\mathcal{E}^2(p,p')$, and found the eigenvalues and eigenvectors of the latter;

5. We kept iterating the process until we obtained convergence of the eigenvalues up to some prescribed precision.

We obtained stable results with an $N = 64$ lattice and 50 iterations. We checked our results with the continuum extrapolated mean field formula of Eq. (4.52) by solving that nonlinear equation with the Mathematica `Solve` function. We found that the Python and Mathematica results agree almost perfectly.

We fix the numerical values of the parameters as follows. We set $\hat{m} = 1$, and considered two values for the inverse temperature, $\hat{\beta} = 1$ and $\hat{\beta} = 0.5$. The first value of $\hat{\beta}$ corresponds to a temperature equal to the mass and the latter to a temperature 2 times larger than the mass. Regarding λ, we want a strong coupling to characterize a nonperturbative situation. Since λ is dimensionful, one needs a criterion to characterize its strength. We assume that $\hat{\lambda}$ characterizes strong coupling if the interaction changes the mass by at least 50% in the mean field approximation, i.e. $m_*/m = 1.5$. We found that, for $\hat{m} = 1$ and $\hat{\beta} = 1$, the value of $\hat{\lambda}$ satisfying that criterion is $\hat{\lambda} \sim 25$. Therefore, we put $\hat{\lambda} = 25$.

In the numerical computations, we used the interval $-\pi/a \leq q \leq \pi/a$ as the set $\mathcal{S}$. This means that all off-diagonal elements of the matrix $\mathcal{E}^2(p,p')$ are nonzero. But, as already mentioned, in view of the limitations of the model and the lack of phenomenological or theoretical guidance on $n(\mathcal{S})$, we simulated its possible effects by changing the weight with which the direct and exchange interactions contribute to $\mathcal{E}^2(p,p')$. The aim of this theoretical experiment is solely to illustrate the impact off diagonal elements with sufficient strength have on the spectrum. We introduced a parameter $1/2 \leq \kappa \leq 1$ that controls that weight, namely: if the interaction contributes with weight κ to the diagonal terms, then it contributes to the off-diagonal terms with weight $1-\kappa$ of the diagonal contribution. The value $\kappa = 1$ leads to the mean field result and for $\kappa < 1/2$ the determinant of the matrix is zero and our code breaks down.

Figure 4.3 displays the eigenvalues $\hat{\omega}^2(k)$ for four values of κ. The two panels differ by the value of the coupling; the right panel is for a coupling twice as big than that of the left panel. The black curve is the eigenvalue of the noninteracting theory, $\lambda = 0$, whereas the red dash-dotted is the mean field (MF) result. A first inspection of the figure reveals that the off diagonal terms indeed impact significantly the energy spectrum. Of course, this is a consequence of our setup and not of the

model. But there is a model feature, not of our setup, in that doubling the coupling, and keeping the same values for $\hat{\beta}$ and κ, does not lead to a substantial change in the spectrum. The numerical data files show that the mass m_* increases by only 10% when one doubles the coupling. This is a feature of the model because one can take the MF analytical formula in Eq. (3.92) and use Mathematica to analyse the results. One finds that as the coupling keeps increasing, there is a saturation effect on the increase of m_*.

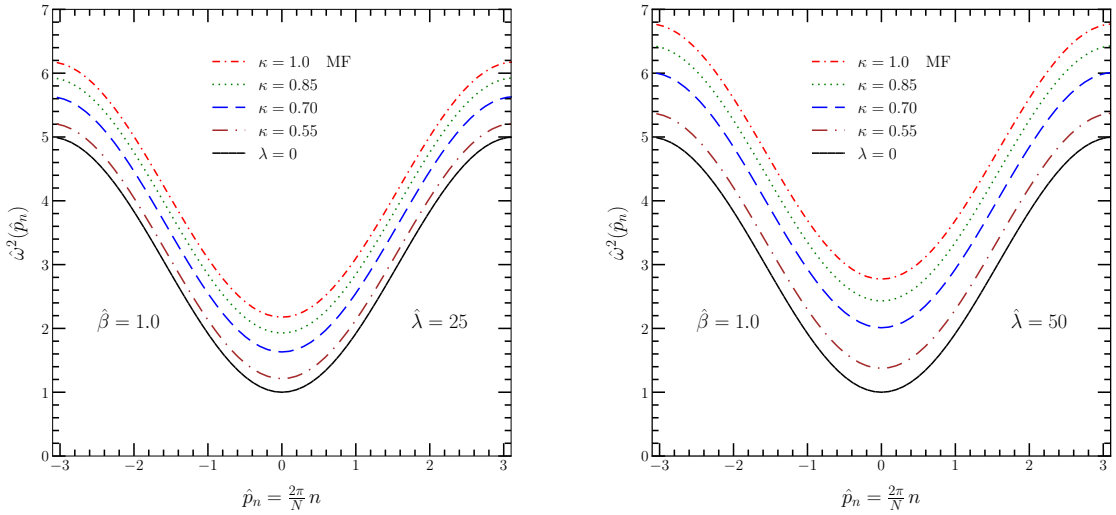

Figure 4.3: The eigenvalues of $\mathcal{E}(p, p')$, Eq. (4.25), for $\hat{m} = 1$ and $N = 64$ lattice sites.

We show the results for the correlation function in Fig. 4.4, for the same set of parameters. We denote by $\hat{D}(\hat{p}_n)$ the lattice version of Eq. (4.45):

$$\hat{D}(\hat{p}_n) = N \sum_m \frac{\phi^*_{\hat{k}_m}(\hat{p}_n)\, \phi_{\hat{k}_m}(\hat{p}_n)}{\hat{\omega}(\hat{k}_m)} \frac{1}{e^{\hat{\beta}\hat{\omega}(\hat{k}_m))} - 1} \,. \tag{4.63}$$

Essentially the same features seen for $\hat{\omega}$ are seen for $\hat{D}$ regarding parameter dependence. As the interaction gets stronger the mass m_* gets larger and the momentum dependence spreads out (in coordinate space it peaks toward the origin). We discussed this feature in Chapter 3, around Eq. (3.78). The more the mass increases, the more classical the system becomes.

For completeness, we repeated the previous computations for a $\hat{\beta} = 0.5$, that is, a temperature two times smaller than of the examples above. We show the results in Figs. 4.5 and 4.6. Nothing changes qualitatively, but there is clear

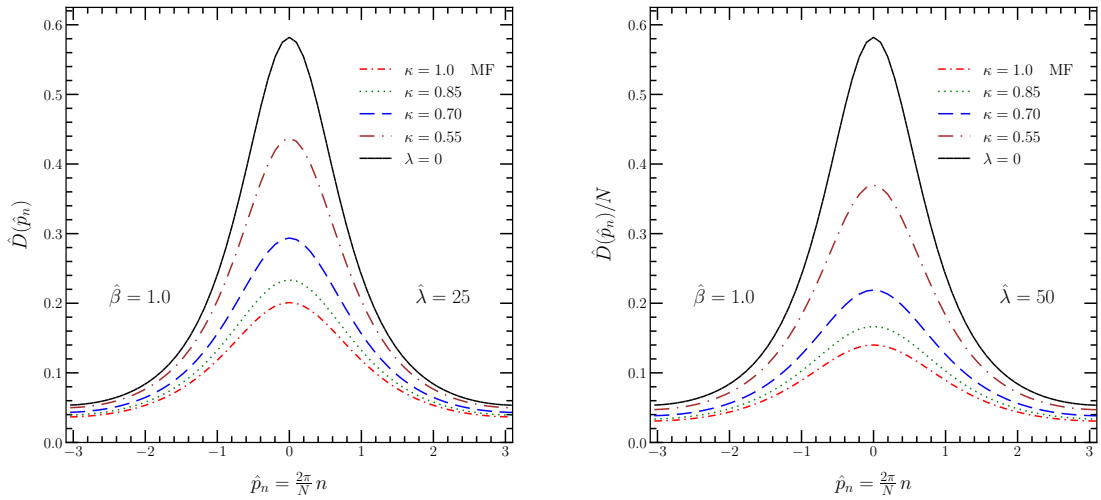

Figure 4.4: The correlation function $\hat{D}(\hat{p}_n)$, Eq. (4.63), for $\hat{m} = 1$ and $N = 64$ lattice sites.

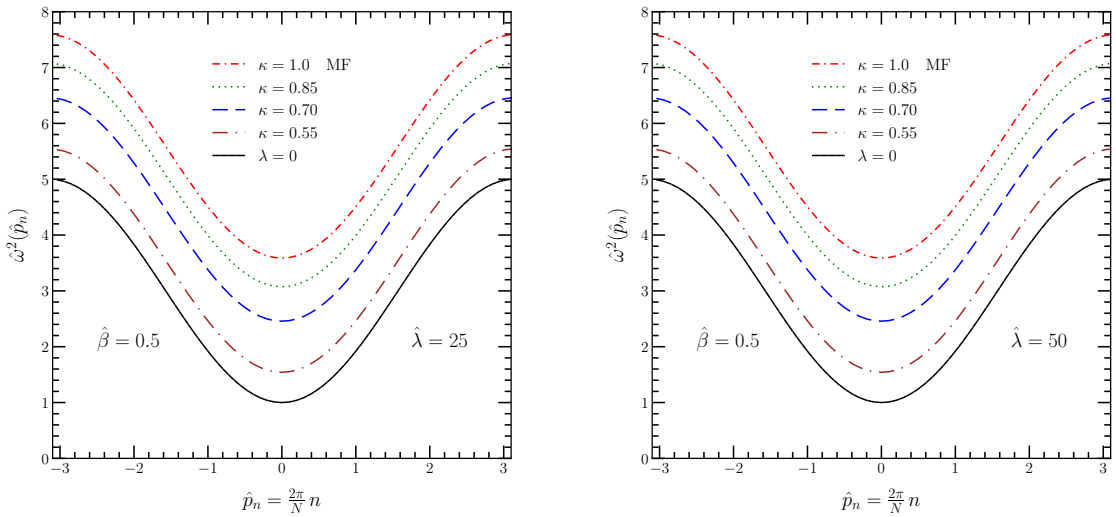

Figure 4.5: Same as in Fig. 4.3, but for $\hat{\beta} = 0.5$.

quantitative impact on both quantities, although it seems larger on the correlation function. The Bose-Einstein distribution involving the product $\hat{\beta}\hat{\omega}$ does not change much, $\hat{\beta}$ decreases by a factor of two but $\hat{\omega}$ concomitantly increases by almost the same factor. The effect on $\hat{D}$ comes from the $1/\hat{\omega}$ in (4.63). The black curve for $\hat{D}$ increases compared to the previous case because it affects the Bose-Einstein distribution, as there is no temperature effect on the noninteracting eigenvalue.

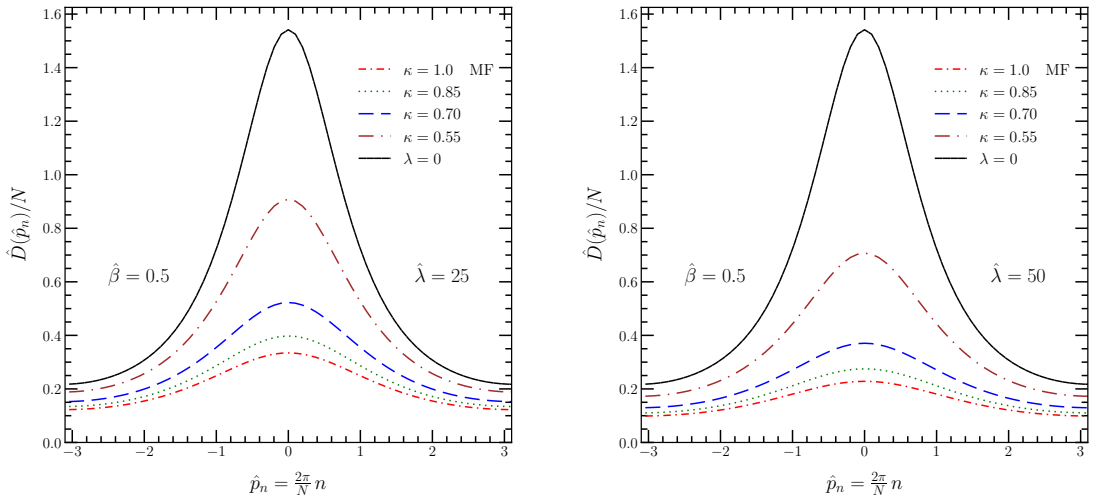

Figure 4.6: Same as in Fig. 4.4, but for $\hat{\beta} = 0.5$.

Table 4.1 displays the results for the 2nd-Rényi entropy $S_2^{(b)}$. Noticeable is the decrease of $S_2^{(b)}$ as $\hat{\lambda}$ increases. This is so because as $\hat{\lambda}$ increases, m_* increases and the more classical the system is becoming. The more classical the system is, the more information one has on the system. Now, the behavior with respect to the temperature is just the opposite, $S_2^{(b)}$ increases with the temperature, as expected. This is expected because the higher the temperature the less information one has on the system.

Table 4.1: The 2nd Rényi entropy $S_2^{(b)}$, Eq. (4.48), for the same values of $\hat{\beta}$ and $\hat{\lambda}$ used in Figs 4.3-4.6.

	$\hat{\beta} = 1.0$		$\hat{\beta} = 0.5$	
κ	$\hat{\lambda} = 25$	$\hat{\lambda} = 50$	$\hat{\lambda} = 25$	$\hat{\lambda} = 50$
1.00	4.5	2.5	10.0	5.4
0.85	5.8	3.5	12.9	7.7
0.70	7.8	5.3	17.7	11.8
0.55	11.9	10.1	28.7	23.6

To conclude, this numerical exercise illustrates the importance of the off diagonal terms of the $\mathcal{E}(p, p')$ for accessing effects beyond the traditional mean field approximation. Additional effects come from the contributions of H' and H''. These contributions are also beyond mean field. Moreover, as remarked earlier, the contributions of H' and H'' are crucial to explore features associated with the negativity of the Wigner functional, since $W_\beta^{(q)}$ is a single Gaussian. We reserve for future work the study of these issues within a more realistic model. For example, complex real fields in dimensions larger than $1+1$-dimensions and fermionic fields are natural candidates for further explorations of the method here developed.

Chapter 5

Conclusion and Perspectives

The primary aim of our study was to construct a formalism to compute corrections to the mean field approximation for the Wigner functional in QFT. To fulfill that aim, we transcribed to the QFT Wigner functional formalism introduced in Ref. [11] the variational method developed in statistical mechanics in Ref. [29]. The starting point of the variational method is to select a number of scattering processes in the Hamiltonian of the model. Those processes should capture most of the physics of the problem at hand and, at the same time, lead to a problem that can be solved by using a combination of the Gibbs variational principle and perturbation theory. The full Hamiltonian was split into a Hamiltonian that is quadratic in the fields, $\hat{H}_q$, and a sum of two nonquadratic Hamiltonians $\hat{H}' + \hat{H}''$. The Hamiltonian $\hat{H}_q$ contains only those selected processes, characterized by the transferred momentum q. $\hat{H}_q$ is diagonalized through a linear unitary transformation that depends on trial gap functions determined by the Gibbs variational principle. The nonquadratic part, that also depends on the trial functions, should be treated by perturbation theory.

The reason for employing the construction of Ref. [11], instead of the more traditional ones [19, 9, 15], was that that construction is a natural generalization of the standard Wigner function in quantum mechanics. Fields and their conjugate momenta are the dynamical variables defining the phase space, instead of the particle coordinates and momenta. As such, many aspects of the standard Wigner function in quantum mechanics are brought into quantum field theory.

The fact that the variational method of Ref. [29] builds on the equilibrium thermal density matrix was key to the construction of a Wigner functional that goes beyond the traditional mean field approximation that keeps only the direct and exchange processes. We believe that we have developed a novel, promising formalism to treat nonperturbative problems in quantum field theory using phase space methods. Although we relied on the self-interacting real scalar quantum field theory in $1+1$ dimensions to set up the variational method, the model served the purpose to reveal general features of the formalism which will be present in

more realistic models. It also allowed us to do a numerical exercise to explore some features of the formalism. We computed with relative ease the spectrum of $\hat{H}_q$ and presented numerical results for interesting quantities, the two-point correlation function and the 2^{nd}-Rényi entropy. Now, it is important to reiterate that for this method to be useful in real applications one needs a good starting point. That is, one needs to have a good idea on what processes to include in $\hat{H}_q$. If the starting point does not capture the main physics of the problem, then too much weight is left for $\hat{H}'$ and $\hat{H}''$ to capture that physics. In such a situation, $\hat{H}'$ and $\hat{H}''$ might not be perturbative.

We did not go very deep into the question on how to implement the perturbative corrections from $\hat{H}'$ and $\hat{H}''$ to the Wigner functional. As mentioned in Chapter 4, one most likely would need to extend to QFT the off-diagonal Wigner function formalism discussed in Ref. [58, 12, 3, 59]. We also envisage the use of the QFT method of Ref. [16], which does not rely on the use of Hilbert space techniques but uses generating functionals. These questions are perspectives for future studies.

The Wigner functional formalism we have used is well suited to employ information theory concepts in quantum field theory. Traditional field theory methods have been used to study e.g. entanglement between two spatial regions [55] and entanglement of field momentum modes [60, 61] in the vacuum. To obtain the vacuum density matrix in our formalism, one needs to take the limit of temperature at the end of the calculation. Taking this limit might not be an easy task when one does not have an analytical result. Nevertheless, one can borrow techniques used to compute entanglement entropies in lattice simulations of quantum field theories [62]. The strategy of approaching vacuum properties starting with a thermal density matrix was recently used to study entanglement entropy with perturbation theory in quantum mechanics [63] and field theory [61]. We envisage great opportunities of using this Wigner functional formalism to tackle such questions. In particular, since the use of the Wigner functional provides a bridge between quantum and classical phase-space physics, it provides the natural framework to address issues related to nonclassicality and decoherence[64] in quantum field theory.

Appendix A

Gaussian Functional Integral

In this appendix we evaluate a general Gaussian integral for the bosonic case treated along this work.

A.1 Simple Case

We start from the general form

$$I = \int Dx\, e^{-x^T M x} = \int Dx\, e^{-\sum_{i,j} x^i M_{ij} x_j}\,, \tag{A.1}$$

where M is an invertible matrix. This leads to

$$I = \prod_i^\infty \int \frac{dx_i}{\sqrt{\pi}}\, e^{-Mx^2}\,, \tag{A.2}$$

since it is implicit that we defined $\int Dx = \prod_i^\infty \int \frac{dx_i}{\sqrt{\pi}}$ with this $\frac{1}{\sqrt{\pi}}$ factor as a mere normalization. Equation (A.2) is an infinity productory of gaussian integrals, that we can evaluate for one dimension as

$$I' = \int dx\, e^{-Mx^2}\,. \tag{A.3}$$

Conveniently squaring this integral leads to

$$I'^2 = \left[\int dx\, e^{-Mx^2}\right]^2 = \int_{R^2} e^{-(x^2+y^2)M}\, dxdy\,. \tag{A.4}$$

No we can changing variables to polar coordinates

$$I'^2 = \int_0^{2\pi} \int_0^\infty e^{-Mr^2} r dr d\theta\,. \tag{A.5}$$

Changing variables again so that $u = r^2$ and $du = 2rdr$ (integration limits remain the same as r)

$$I'^2 = \frac{1}{2}\int_0^{2\pi}\int_0^{\infty} e^{-Mu} du d\theta = \frac{1}{2}\int_0^{2\pi} d\theta \left[-\frac{e^{-Mu}}{M}\right]_0^{\infty} = \frac{1}{2}2\pi\frac{1}{M} = \frac{\pi}{M}, \tag{A.6}$$

so, taking the square root

$$I' = \sqrt{\frac{\pi}{M}}. \tag{A.7}$$

The generalization of this result to infinity integrals where M must be a diagonal matrix:

$$I = \prod_i^{\infty}\int \frac{dx_i}{\sqrt{\pi}} e^{-Mx^2} = \sqrt{\frac{1}{\det[M]}} \tag{A.8}$$

A.2 General Case

The general case of such functional integrals is the field version deformed by a source term so that

$$I = \int_{-\infty}^{\infty} \frac{d\phi(x)}{\sqrt{\pi}}\, e^{-a(x)\phi^2(x)+b(x)\phi(x)}. \tag{A.9}$$

We drop the argument in the equation now on to easy notation, unless necessary. In order to compute such integral we need to complete the square of the argument of exponential

$$I = \int_{-\infty}^{\infty} \frac{d\phi}{\sqrt{\pi}} e^{-a(\phi-\frac{b}{2a})^2+\frac{\phi}{4a}}, \tag{A.10}$$

then we shift the integrand variable $\phi(x) \longrightarrow \phi(x) - \frac{b(x)}{2a(x)}$. The Jacobian is obviously 1 because such shift does not change the integration measure,

$$I = e^{\frac{|b|^2}{4a}} \int_{-\infty}^{\infty} \frac{d\phi}{\sqrt{\pi}} e^{-a\phi^2}. \tag{A.11}$$

Now we use the same trick as before and get

$$I = e^{\frac{|b|^2}{4a}} \sqrt{\frac{1}{a}}. \tag{A.12}$$

The generalization to multidimensional integrals needs a generelization of the variable ϕ so that $a\phi^2 \longrightarrow \phi_i^*\, a_{ij}\, \phi_j = \phi^\dagger \mathbf{a}\phi$. After diagonalizing $\mathbf{a}$ the integral

becomes a product of one-dimensional Gaussian integrals over $\phi(x_i)$, with a being replaced by an eigenvalue of **a**:

$$\begin{aligned}\int D\phi\, e^{-\phi^\dagger\, a\, \phi + b\, \phi} &= \int_{-\infty}^{\infty} d\phi(x_1)\, \exp\Big[-\phi^\dagger(x_1)\, a(x_1)\, \phi(x_1) + b(x_1)\phi(x_1)\Big] \\ &\quad \times \int_{-\infty}^{\infty} d\phi(x_2)\, \exp\Big[-\phi^\dagger(x_2)\, a(x_2)\, \phi(x_2) + b(x_2)\phi(x_2)\Big] \\ &\quad \times \cdots \int_{-\infty}^{\infty} d\phi(x_n)\, \exp\Big[-\phi^\dagger(x_n)\, a(x_n)\, \phi(x_n) + b(x_n)\phi(x_n)\Big] \\ &= e^{-\frac{|b|^2}{4a}} \prod_x^{\infty} \sqrt{\frac{\pi}{a(x)}}\,, \end{aligned} \tag{A.13}$$

where it is understood that $D\phi(x) = \prod_x^{\infty} \frac{d\phi(x)}{\sqrt{\pi^n}}$.

Appendix B

Discretization of the Hamiltonian

We start from the expression for the Hamiltonian in the continuum of the model, Eq. (3.54) with $\mathcal{L}_I(\hat{\Phi}) = -\frac{\lambda}{4!}\hat{\Phi}^4$:

$$\hat{H} = \hat{H}_0 + \hat{H}_I, \tag{B.1}$$

with

$$\hat{H}_0 = \frac{1}{2}\int dx \left[\hat{\Pi}^2(x) - \hat{\Phi}(x)\nabla^2\hat{\Phi}(x) + m^2\hat{\Phi}^2(x)\right], \tag{B.2}$$

$$\hat{H}_I = \frac{\lambda}{4!}\int dx\, \hat{\Phi}^4. \tag{B.3}$$

The term with the Laplacian comes from an integration by parts. We employ a one dimensional quantization box of length L and impose periodic boundary conditions on the fields. As mentioned in the main text, we can maintain the spatial coordinate x continuous, or discretize it by using a lattice. We start with continuous x.

The periodic boundary conditions imply that the momentum is discrete:

$$p_n = \frac{2\pi}{L}n, \quad n = 0, \pm1, \pm2, \ldots. \tag{B.4}$$

The fields $\hat{\Phi}(x)$ and $\hat{\Pi}(x)$ are written in a Fourier series:

$$\begin{pmatrix} \hat{\Phi}(x) \\ \hat{\Pi}(x) \end{pmatrix} = \frac{1}{L}\sum_n e^{ip_n x} \begin{pmatrix} \hat{\Phi}(p) \\ \hat{\Pi}(p) \end{pmatrix}. \tag{B.5}$$

Replacing these series in Eq. (B.2), one obtains

$$\hat{H}_0 = \frac{1}{2L}\sum_p \hat{\Pi}^\dagger(p)\,\hat{\Pi}(p) + \frac{1}{2L}\sum_p (p^2 + m^2)\,\hat{\Phi}^\dagger(p)\,\hat{\Phi}(p), \tag{B.6}$$

where we omitted the index n of p_n to conform with the expression given in

the main text, Eq. (4.3). To obtain this result, we used $\hat{\Phi}(-p) = \hat{\Phi}^\dagger(p)$ and $\hat{\Pi}(-p) = \hat{\Pi}^\dagger(p)$, and also

$$\int_{-L}^{L} dx\, e^{-i(p_n + p_{n'})x} = L\,\delta_{n,-n'}\,. \tag{B.7}$$

For the $\hat{H}_I$, we obtain:

$$\hat{H}_I = \frac{\lambda}{4!}\frac{1}{L^4}\sum_{n_1,\ldots,n_4} \hat{\Phi}(p_{n_4})\hat{\Phi}(p_{n_3})\hat{\Phi}(p_{n_1})\hat{\Phi}(p_{n_2})\, L\,\delta_{p_{n_1}+p_{n_2},-p_{n_3}-p_{n_4}}\,, \tag{B.8}$$

where we have used again Eq. (B.7). If we choose to eliminate p_{n_4} using the Kronecker delta, $p_{n_4} = -p_{n_1} - p_{n_2} - p_{n_3}$, we obtain:

$$\begin{aligned}
\hat{H}_I &= \frac{\lambda}{4!}\frac{1}{L^3}\sum_{n_1,n_2,n_3} \hat{\Phi}(-p_{n_1} - p_{n_2} - p_{n_3})\hat{\Phi}(p_{n_3})\hat{\Phi}(p_{n_2})\hat{\Phi}(p_{n_1}) \\
&= \frac{\lambda}{4!}\frac{1}{L^3}\sum_{n_1,n_2,n_3} \hat{\Phi}^\dagger(p_{n_1} + p_{n_2} + p_{n_3})\hat{\Phi}(p_{n_3})\hat{\Phi}(p_{n_2})\hat{\Phi}(p_{n_1}) \\
&= \frac{\lambda}{4!}\frac{1}{L^3}\sum_{n_1,n_2,n_3} \hat{\Phi}^\dagger(p_{n_1} + p_{n_2} - p_{n_3})\hat{\Phi}^\dagger(p_{n_3})\hat{\Phi}(p_{n_2})\hat{\Phi}(p_{n_1})\,,
\end{aligned} \tag{B.9}$$

where we made $p_{n_3} \to -p_{n_3}$ in the last step. Now changing $p_{n_1} - p_{n_3} = q$ we end up with

$$\hat{H}_I = \frac{\lambda}{4!}\frac{1}{L^3}\sum_{p,p',q} \hat{\Phi}^\dagger(p'+q)\hat{\Phi}^\dagger(p-q)\hat{\Phi}(p)\hat{\Phi}(p')\,, \tag{B.10}$$

where again we omitted the discrete indices to conform with the expression in the main text, Eq. (4.4).

Next, we consider discrete x on a lattice [43] with N sites, such that $x \to x_l = la$, $l = 0, 1, \ldots, N-1$, where a is the lattice spacing and $L = Na$. To Fourier transform, there must be exactly the same number of momentum values; we choose them symmetrically as:

$$n = -N/2 + 1, \ldots, 0, \ldots N/2\,. \tag{B.11}$$

The the possible values of the momentum in the infinite volume limit, $N \to \infty$ and a fixed, are then:

$$-\frac{\pi}{a} \le p \le +\frac{\pi}{a}\,. \tag{B.12}$$

This is so because the shortest wave length is $\lambda_{min} = 2a$ and the largest momentum

p_{max} is then (recall we are using $\hbar = 1$):

$$p_{max} = \frac{2\pi}{\lambda_{min}} = \frac{\pi}{a}\,. \tag{B.13}$$

For the discretization of the Laplacian we use the standard central difference formula:

$$\nabla^2\Phi(x) \to \frac{\Phi(x+a) - 2\Phi(x) - \Phi(x-a)}{a^2}\,. \tag{B.14}$$

This leads to

$$\begin{aligned}\int dx\,\Phi(x)\nabla^2\Phi(x) \;\to\; & a\sum_l \frac{1}{a^2}\frac{1}{(Na)^2}\sum_{nn'}\Phi(n')\Phi(n)e^{i\frac{2\pi}{N}n'l} \\ & \times\left(e^{i\frac{2\pi}{N}n(l+1)} - 2e^{i\frac{2\pi}{N}nl} + e^{i\frac{2\pi}{N}n(l-1)}\right) \\ = \;& -\frac{1}{N^2a^3}\sum_{nn'} 4\sin^2\left(\frac{\pi}{N}n\right)\Phi(n')\Phi(n)\sum_l e^{i\frac{2\pi}{N}(n'+n)l}\,. \end{aligned} \tag{B.15}$$

Next, we use here the result [43]:

$$r = e^{i\frac{2\pi}{N}(n-n')} \to \frac{1}{N}\sum_{l=0}^{N-1} r^l = \frac{1}{N}\frac{1-r^N}{1-r} = \delta_{n,n'}\,, \tag{B.16}$$

to obtain:

$$\int dx\,\Phi(x)\nabla^2\Phi(x) \;\to\; -\frac{1}{Na}\sum_n \Phi^\dagger(n)\,\frac{4}{a^2}\sin^2\left(\frac{\pi}{N}n\right)\Phi(n)\,, \tag{B.17}$$

where we used $\Phi(-n) = \Phi^\dagger(n)$.

The mass and interaction terms of the Hamiltonian have the same structure as in the previous discretization. This establishes the results shown in Eqs (4.3) and (4.4), with the two momentum discretization schemes distinguished by $\bar{p}$ given in Eq. (4.5).

Appendix C

Wigner Functional in Phase Space

C.1 Expectation Values

In this section we aim to prove Eqs. (3.50) and (3.51). We start from the definition of Z in Eq. (3.51):

$$Z = \mathrm{Tr}\ \hat{\rho}(t). \tag{C.1}$$

The aim is to express the trace in terms of the Wigner functional $W[\Phi, \Pi; t]$. We compute the trace in the basis of the eigenstates of $\hat{\Phi}(x)$:

$$\hat{\Phi}(x)\,|\Phi\rangle = \Phi(x)\,|\Phi\rangle\,. \tag{C.2}$$

Equation (C.1) is then given by the path integral

$$Z = \mathrm{Tr}\ \hat{\rho}(t) = \int D\Phi(x)\,\langle\Phi(x)|\hat{\rho}|\Phi(x)\rangle\,, \tag{C.3}$$

which we rewrite as

$$\begin{aligned} Z &= \int D\Phi(x) D\varphi(x)\,\delta(\varphi(x))\left\langle \Phi(x)+\frac{\varphi(x)}{2}\middle|\hat{\rho}(t)\middle|\Phi(x)-\frac{\varphi(x)}{2}\right\rangle \\ &= \int D\Phi(x) D\varphi(x)\frac{D\Pi(x)}{2\pi}\,e^{-i\int dx\,\Pi(x)\varphi(x)} \\ &\quad\times\left\langle \Phi(x)+\frac{\varphi(x)}{2}\middle|\hat{\rho}(t)\middle|\Phi(x)-\frac{\varphi(x)}{2}\right\rangle, \end{aligned} \tag{C.4}$$

in which we used the fact that

$$\delta(\varphi(x)) = \int \frac{D\Pi(x)}{2\pi}\,e^{-i\int dx\,\Pi(x)\varphi(x)}\,. \tag{C.5}$$

The desired result follows trivially, as one can identify the Wigner functional as the functional integral over φ and rewrite Z as:

$$Z = \int D\Phi(x) \frac{D\Pi(x)}{2\pi} W[\Phi, \Pi, t] \,. \tag{C.6}$$

Next, we prove Eq. (3.50) for the case $\hat{\mathcal{O}}(\hat{\Pi})$. Again, we start computing the trace in the basis of the eigenstates of $\hat{\Phi}(x)$ and make the same tricks made above with respect to the insertion of a $\delta(\varphi(x))$ functional followed by the field shift $\Phi(x) \to \Phi(x) - \varphi(x)/2$ (to avoid clutter we drop in some places the x dependence in the field operators):

$$\langle \hat{\mathcal{O}}(\hat{\Pi}) \rangle = \frac{1}{Z} \int D\Phi D\varphi \frac{D\Pi}{2\pi} e^{-i\int dx\, \Pi(x)\varphi(x)} \langle \Phi + \frac{\varphi}{2} | \hat{\rho}(t) \hat{\mathcal{O}}(\hat{\Pi}) | \Phi - \frac{\varphi}{2} \rangle \,. \tag{C.7}$$

Next, we insert the completeness relation of the momentum field operator $\hat{\Pi}(x)$ eigenfunctions $|\Pi(x)\rangle$, namely

$$\mathbb{1} = \int D\Pi \, |\Pi\rangle\langle\Pi| \,, \tag{C.8}$$

to obtain

$$\begin{aligned} \langle \hat{\mathcal{O}}(\hat{\Pi}) \rangle = \frac{1}{Z} \int D\Phi D\varphi \frac{D\Pi}{2\pi} \int \frac{D\Pi_1}{2\pi} \frac{D\Pi_2}{2\pi} e^{-i\int dx\, \Pi(x)\varphi(x)} \\ \times \langle \Phi + \frac{\varphi}{2} | \Pi_1 \rangle \, \langle \Pi_1 | \hat{\rho}(t) \hat{\mathcal{O}}(\hat{\Pi}) | \Pi_2 \rangle \, \langle \Pi_2 | \Phi - \frac{\varphi}{2} \rangle \,, \end{aligned} \tag{C.9}$$

where the factor 2π was put in for convenience of comparison with Ref. [11]. Then, we use the (unnormalized) relation

$$\langle \Phi | \Pi \rangle = e^{-i\int dx \Pi(x)\Phi(x)} \,, \tag{C.10}$$

to write

$$\langle \Phi + \frac{\varphi}{2} | \Pi_1 \rangle = e^{i\int dx \left[\Pi_1(x)\Phi(x) + \frac{\Pi_1\varphi}{2}\right]} \,, \tag{C.11}$$

$$\langle \Pi_2 | \Phi - \frac{\varphi}{2} \rangle = e^{-i\int dx \left[\Pi_2(x)\Phi(x) - \frac{\Pi_2\varphi}{2}\right]} \tag{C.12}$$

so that one can express $\langle\hat{\mathcal{O}}(\hat{\Pi})\rangle$ as

$$\begin{aligned}\langle\hat{\mathcal{O}}(\hat{\Pi})\rangle &= \frac{1}{Z}\int D\Phi D\varphi\frac{D\Pi}{2\pi}\frac{D\Pi_1}{2\pi}\frac{D\Pi_2}{2\pi}\,e^{-i\int dx\Pi(x)\varphi(x)}\;\mathcal{O}(\Pi_2)\\ &\quad\times\exp\Big\{i\int dx\Big[(\Pi_1-\Pi_2)\Phi+\frac{1}{2}(\Pi_1+\Pi_2)\varphi\Big]\Big\}\langle\Pi_1|\hat{\rho}(t)|\Pi_2\rangle\,.\end{aligned}$$

Now, we observe that

$$\begin{aligned}&\mathcal{O}(\Pi_2)\,\exp\Big\{i\int dx\Big[(\Pi_1-\Pi_2)\Phi+\frac{1}{2}(\Pi_1+\Pi_2)\varphi\Big]\Big\}\\ &=\mathcal{O}\Big(\frac{1}{i}\frac{\delta}{\delta\varphi(x)}-\frac{1}{2i}\frac{\delta}{\delta\Phi(x)}\Big)\exp\Big\{i\int dx\Big[(\Pi_1-\Pi_2)\Phi+\frac{1}{2}(\Pi_1+\Pi_2)\varphi\Big]\Big\}\,.\end{aligned}\tag{C.13}$$

Then we integrate partially in $\varphi(x)$ to obtain

$$\begin{aligned}\langle\hat{\mathcal{O}}(\hat{\Pi})\rangle &= \frac{1}{Z}\int D\Phi D\varphi\frac{D\Pi}{2\pi}\frac{D\Pi_1}{2\pi}\frac{D\Pi_2}{2\pi}\,e^{-i\int dx\Pi(x)\varphi(x)}\mathcal{O}\Big(\Pi-\frac{1}{2i}\frac{\delta}{\delta\Phi(x)}\Big)\\ &\quad\times\exp\Big\{i\int dx\Big[(\Pi_1-\Pi_2)\Phi+\frac{1}{2}(\Pi_1+\Pi_2)\varphi\Big]\Big\}\langle\Pi_1|\hat{\rho}(t)|\Pi_2\rangle\,.\end{aligned}$$

A further partial integration in Φ amounts to put $\mathcal{O}\big(\Pi-(1/2i)\delta/\delta\Phi\big)=\mathcal{O}(\Pi)$ because the functional derivative $\delta/\delta\Phi(x)$ acting on $\exp(-i\int dx\Pi(x)\varphi(x))$ vanishes. Therefore, one obtains the desired result:

$$\begin{aligned}\langle\hat{\mathcal{O}}(\hat{\Pi})\rangle &= \frac{1}{Z}\int D\Phi D\varphi\frac{D\Pi}{2\pi}\int\frac{D\Pi_1}{2\pi}\frac{D\Pi_2}{2\pi}\,e^{-i\int dx\,\Pi(x)\varphi(x)}\\ &\quad\times\mathcal{O}(\Pi)\;\langle\Phi+\frac{\varphi}{2}|\Pi_1\rangle\,\langle\Pi_1|\hat{\rho}(t)|\Pi_2\rangle\,\langle\Pi_2|\Phi-\frac{\varphi}{2}\rangle\\ &= \frac{1}{Z}\int D\Phi\frac{D\Pi}{2\pi}\int D\varphi\,e^{-i\int dx\,\Pi(x)\varphi(x)}\langle\Phi+\frac{\varphi}{2}|\rho(t)\mathcal{O}(\Pi)|\Phi-\frac{\varphi}{2}\rangle\\ &= \frac{1}{Z}\int D\Phi\frac{D\Pi}{2\pi}\;\mathcal{O}(\Pi)\;W(\Phi(x),\Pi(x))\,.\end{aligned}\tag{C.14}$$

The case in which $\hat{O}(\hat{\Phi})$ is straightforward, similar to the demonstration of the result for Z. The situation gets a little more complicated for $\hat{\mathcal{O}}(\hat{\Phi}(x),\hat{\Pi}(x))$ because the operators $\hat{\Phi}(x)$ and $\hat{\Pi}(x)$ do not commute. A direct computation shows

$$\Big\langle\hat{\Pi}(x)\hat{\Phi}(y)\Big\rangle=\Big\langle\Pi(x)\Phi(y)\Big\rangle-\frac{i}{2}\delta(x-y)\,,\tag{C.15}$$

while

$$\left\langle \hat{\Phi}(y)\hat{\Pi}(x)\right\rangle = \left\langle \Pi(x)\Phi(y)\right\rangle + \frac{i}{2}\delta(x-y)\,, \tag{C.16}$$

so

$$\left\langle \left\{\hat{\Pi}(x),\,\hat{\Phi}(y)\right\}\right\rangle = \left\langle \Pi(x)\Phi(y)\right\rangle, \tag{C.17}$$

where the anticommutator is defined as $\{\hat{A},\hat{B}\} \equiv \frac{1}{2}(\hat{A}\hat{B}+\hat{B}\hat{A})$. If we generalize this result above we prove the equality $\langle\hat{\mathcal{O}}(\hat{\Phi},\hat{\Pi})\rangle = \langle\mathcal{O}(\Phi,\Pi)\rangle$ assuming that the pair of non-commuting operators are symmetrized.

To conclude this part, we mention that similar results hold when using the field operators in momentum space. The only difference is that one has to integrate over real and imaginary parts of the field operators and be careful in not overcounting degrees of freedom due to the constraint $\Phi^*(p) = \Phi(-p)$ (and of course $\Pi^*(p) = \Pi(-p)$).

C.2 Equation of Motion

We want to prove Eq. (3.55). We separate the Hamiltonian of Eq. (3.54) in several parts, naming them $\hat{H}_\Pi$, $\hat{H}_\nabla$, $\hat{H}_m$ and $\hat{H}_I$. The contribution of each one to the equation of motion is G_Π, G_∇, G_m and G_I, respectively.

$$G_i = \int D\varphi\, \exp\Big[-i\int dx\,\Pi(x)\varphi(x)\Big]\langle\Phi(x)+\frac{\varphi}{2}\,|\,\Big[\hat{H}_i,\,\hat{\rho}\Big]\,|\,\Phi(x)-\frac{\varphi}{2}\rangle\,. \tag{C.18}$$

We start by $\hat{H}_m = \frac{m^2}{2}\hat{\Phi}^2$

$$\begin{aligned} G_m &= \frac{m^2}{2}\int dx\int D\varphi\, e^{-i\int dx\Pi(x)\varphi(x)}\langle\Phi(x)+\frac{\varphi}{2}\,|\,\hat{\Phi}^2\hat{\rho}-\hat{\rho}\hat{\Phi}^2\,|\,\Phi(x)-\frac{\varphi}{2}\rangle \\ &= \frac{m^2}{2}\int dx\int D\varphi\, e^{-i\int dx\Pi(x)\varphi(x)}\Big(\Big|\Phi(x)+\frac{\varphi}{2}\Big|^2-\Big|\Phi(x)-\frac{\varphi}{2}\Big|^2\Big) \\ &\quad\times\langle\Phi(x)+\frac{\varphi}{2}\,|\,\hat{\rho}\,|\,\Phi(x)-\frac{\varphi}{2}\rangle\,, \end{aligned} \tag{C.19}$$

now using that $\varphi\, e^{-i\int dx\Pi(x)\varphi(x)} = i\hbar\frac{\delta}{\delta\Pi}\, e^{-i\int dx\Pi(x)\varphi(x)}$

$$\begin{aligned} G_m &= m^2 i\hbar\int dx\,\Phi(x)\,\frac{\delta}{\delta\Pi}\int D\varphi\, e^{-i\int dx\Pi(x)\varphi(x)}\langle\Phi(x)+\frac{\varphi}{2}\,|\,\hat{\rho}\,|\,\Phi(x)-\frac{\varphi}{2}\rangle \\ &= i\hbar m^2\int dx\,\Phi(x)\,\frac{\delta}{\delta\Pi}\int D\varphi\, e^{-i\int dx\Pi(x)\varphi(x)}W(\Pi,\Phi;t)\,. \end{aligned} \tag{C.20}$$

The G_I case is immediate demanding that $\hat{\mathcal{L}}(\Phi)$ is a polinomial in Φ and $\varphi\, e^{-i\int dx\Pi(x)\varphi(x)} = i\hbar\frac{\delta}{\delta\Pi}\, e^{-i\int dx\Pi(x)\varphi(x)}$. We follow the same steps toward

$$G_I = -\int dx \left[\hat{\mathcal{L}}\Big(\Phi + \frac{i\hbar}{2}\frac{\delta}{\delta\Pi}\Big) - \hat{\mathcal{L}}\Big(\Phi - \frac{i\hbar}{2}\frac{\delta}{\delta\Pi}\Big)\right] W(\Pi,\Phi;t)\,. \tag{C.21}$$

In the G_Π case we need to introduce two momentum identities

$$\begin{aligned} G_\Pi = \frac{1}{2}\int dx \int D\varphi\, \frac{D\Pi_1}{2\pi}\,\frac{D\Pi_1}{2\pi} e^{-i\int dx\,\Pi(x)\varphi(x)}\,(\,\Pi_1^2(x) - \Pi_2^2(x)\,) \\ \times\langle\,\Phi + \frac{\varphi}{2}\,|\Pi_1\rangle\langle\Pi_1\,|\,\hat\rho\,|\Pi_2\rangle\langle\Pi_2\,|\,\Phi - \frac{\varphi}{2}\rangle\,, \end{aligned} \tag{C.22}$$

then remembering that $\langle\Phi|\Pi\rangle = e^{i\int dx\,\Phi(x)\Pi(x)}$ we can rewrite it as

$$\begin{aligned} G_\Pi \;=\; & \frac{1}{2}\int dx \int D\varphi\, \frac{D\Pi_1}{2\pi}\,\frac{D\Pi_1}{2\pi} e^{-i\int dx\,\Pi(x)\varphi(x)}\,\frac{2\hbar^2}{i^2}\frac{\delta}{\delta\Phi}\frac{\delta}{\delta\varphi} \\ & \times\exp\Big\{\frac{i}{\hbar}\int dx\,\Big[(\,\Pi_1 - \Pi_2\,)\Phi + \frac{1}{2}(\,\Pi_1 + \Pi_2\,)\varphi\Big]\Big\}\langle\Pi_1\,|\hat\rho|\,\Pi_2\rangle \end{aligned} \tag{C.23}$$

Partial integrating in φ

$$\begin{aligned} G_\Pi = -\hbar^2\int dx \int D\varphi\, \frac{D\Pi_1}{2\pi}\,\frac{D\Pi_1}{2\pi}\,\Big[\frac{i}{\hbar}\Pi(x)\, e^{-i\int dx\,\Pi(x)\varphi(x)}\Big] \\ \times\frac{\delta}{\delta\Phi}\,\exp\Big\{\frac{i}{\hbar}\int dx\,\Big[(\,\Pi_1 - \Pi_2\,)\Phi + \frac{1}{2}(\,\Pi_1 + \Pi_2\,)\varphi\Big]\Big\}\langle\Pi_1\,|\hat\rho|\,\Pi_2\rangle\,. \end{aligned} \tag{C.24}$$

Now we can restore the identities in the previous expression

$$\begin{aligned} G_\Pi = -i\hbar\int dx \int D\varphi\, \frac{D\Pi_1}{2\pi}\,\frac{D\Pi_1}{2\pi}\,\Pi(x)\,\frac{\delta}{\delta\Phi}\, e^{-i\int dx\,\Pi(x)\varphi(x)} \\ \times\langle\Phi + \frac{\varphi}{2}\,|\,\Pi_1\rangle\langle\Pi_1\,|\hat\rho|\,\Pi_2\rangle\langle\Pi_2\,|\,\Phi - \frac{\varphi}{2}\rangle\,, \end{aligned} \tag{C.25}$$

and taking off the identities

$$\begin{aligned} G_\Pi \;&=\; -i\hbar\int dx\,\Pi(x)\,\frac{\delta}{\delta\Phi}\int D\varphi\, e^{-i\int dx\,\Pi(x)\varphi(x)}\langle\Phi + \frac{\varphi}{2}\,|\,\hat\rho\,|\,\Phi - \frac{\varphi}{2}\rangle \\ &=\; -i\hbar\int dx\,\Pi(x)\,\frac{\delta}{\delta\Phi}\,W(\Pi,\Phi;t)\,. \end{aligned} \tag{C.26}$$

Finally, to evaluate the G_∇ term we first discretize $\Phi(x)$ in a lattice so that

$$\hat{H}_\nabla = [\nabla\Phi]^2 \longrightarrow \frac{a}{2}\sum_i \left[\frac{\hat{\Phi}_{i+1}-\hat{\Phi}_i}{a}\right]^2 , \tag{C.27}$$

so

$$\begin{aligned} G_\nabla &= \frac{a}{2}\int dx \int D\varphi\, e^{-\frac{i}{\hbar}\int \Pi\varphi} \sum_i \left[\frac{\Phi_{i+1}+\frac{\varphi_{i+1}}{2}-\Phi_i-\frac{\varphi_i}{2}}{a}\right]^2 \\ &\quad - \left[\frac{\Phi_{i+1}-\frac{\varphi_{i+1}}{2}-\Phi_i+\frac{\varphi_i}{2}}{a}\right]^2 \langle\Phi+\frac{\varphi}{2}|\,\hat{\rho}\,|\Phi-\frac{\varphi}{2}\rangle\,. \end{aligned} \tag{C.28}$$

Using that $\varphi\, e^{-\frac{i}{\hbar}\int dx\,\Pi\varphi} = i\hbar\frac{\delta}{\delta\Pi}e^{-\frac{i}{\hbar}\int dx\,\Pi\varphi}$ and after some manipulations

$$G_\nabla = i\hbar\sum_i \frac{\Phi_{i+1}-\Phi_i}{a}\left[\frac{\partial}{\partial\Pi_{i+1}}-\frac{\partial}{\partial\Pi_i}\right] W(\Pi_j,\Phi_j;t)\,, \tag{C.29}$$

multiplying by a/a

$$G_\nabla = i\hbar a\sum_i \frac{\Phi_{i+1}-\Phi_i}{a^2}\left[\frac{\partial}{\partial\Pi_{i+1}}-\frac{\partial}{\partial\Pi_i}\right] W(\Pi_j,\Phi_j;t)\,, \tag{C.30}$$

and we can perform the limit to continuum making $a \longrightarrow 0$; recognizing the derivatives

$$G_\nabla = i\hbar\int dx\,\nabla\Phi\nabla\frac{\delta}{\delta\Pi}W(\Pi,\Phi;t)\,, \tag{C.31}$$

and finally, partially integrating

$$G_\nabla = -i\hbar\int dx\,\nabla^2\Phi\frac{\delta}{\delta\Pi}W(\Pi,\Phi;t)\,. \tag{C.32}$$

Collecting all terms and gluing them together we find Eq. (3.55)

$$\left\{\frac{\partial}{\partial t}+\int dx\left[\Pi(x)\frac{\delta}{\delta\Phi(x)}-\left(m^2\Phi(x)-\nabla^2\Phi(x)\right)\frac{\delta}{\delta\Pi(x)}+\mathcal{K}_I(x)\right]\right\} W[\Phi,\Pi,t]=0\,. \tag{C.33}$$

C.3 Proofs of Results Involving the Thermal Wigner Functional

C.3.1 Wigner Functional for Thermal Equilibrium

In this section we aim to prove Eq. (3.65). We use Eq. (3.64) for the free Hamiltonian $\hat{H}_0$ in Eq. (3.48) that defines the momentum space Wigner functional:

$$\begin{aligned}\widetilde{W}_\beta^{(0)}[\Phi,\Pi] &= \frac{1}{Z^{(0)}}\int D\varphi\, e^{-i\frac{1}{2}\int_{-\infty}^{\infty}\frac{dp}{2\pi}\,[\Pi^*(p)\varphi(p)+\Pi(p)\varphi^*(p)]} \\ &\times\left\langle\Phi+\frac{\varphi}{2}\middle|e^{-\beta\int_{-\infty}^{\infty}\frac{dp}{2\pi}\,\frac{1}{2}\left[\hat{\Pi}^\dagger(p)\hat{\Pi}(p)+(p^2+m^2)\hat{\Phi}^\dagger(p)\hat{\Phi}(p)\right]}\middle|\Phi-\frac{\varphi}{2}\right\rangle. \qquad \text{(C.34)}\end{aligned}$$

Here we wrote the momentum integrals from $-\infty$ to ∞ because the restriction to field variables with momenta $p>0$, to avoid double counting, applies to the fields' real and imaginary parts. Therefore, expressing the field variables in terms of their real and imaginary parts and restricting the momentum integrals to $0\le p<\infty$, we can write $\widetilde{W}_\beta^{(0)}[\Phi,\Pi]$ as

$$\begin{aligned}\widetilde{W}_\beta^{(0)}[\Phi,\Pi] &= \frac{1}{Z^{(0)}}\int D\varphi_R\, D\varphi_I\, e^{-i\int_0^{\infty}\frac{dp}{2\pi}\,[\Pi_R(p)\varphi_R(p)+\Pi_I(p)\varphi_I(p)]} \\ &\times\left\langle\Phi_R+\frac{\varphi_R}{2}\middle|e^{-\beta\int_0^{\infty}\frac{dp}{2\pi}\,\frac{1}{2}\left[\hat{\Pi}_R^2+(p^2+m^2)\hat{\Phi}_R^2\right]}\middle|\Phi_R-\frac{\varphi_R}{2}\right\rangle \\ &\times\left\langle\Phi_I+\frac{\varphi_I}{2}\middle|e^{-\beta\int_0^{\infty}\frac{dp}{2\pi}\,\frac{1}{2}\left[\hat{\Pi}_I^2+(p^2+m^2)\hat{\Phi}_I^2\right]}\middle|\Phi_I-\frac{\varphi_I}{2}\right\rangle. \qquad \text{(C.35)}\end{aligned}$$

We perform the path integral by discretizing the momentum integrals into sums with periodic boundary conditions and using Eqs. (2.52)-(2.54) to compute the expectation values. Specifically:

$$p\to p_n=\frac{2\pi}{L}n \quad \text{with} \quad n=0,\pm1,\pm2,\dots, \qquad \text{(C.36)}$$

$$\int_{-\infty}^{\infty}\frac{dp}{2\pi}\,f(p)\to\frac{1}{L}\sum_{p_n}f(p_n), \qquad \text{(C.37)}$$

$$\langle\Phi'|\cdots|\Phi\rangle\to\prod_p\langle\Phi'(p)|\cdots|\Phi(p)\rangle. \qquad \text{(C.38)}$$

This transforms the path integral into a product of ordinary integrals, effectively

transforming the computation of the Wigner functional into the computation of a Wigner function for each momentum mode p characterized by a coordinate $\hat{\Phi}(p)$ and associated momentum $\hat{\Pi}(p)$. Moreover, the Hamiltonian for each momentum mode resembles that of the harmonic oscillator (HO) and we can use the known HO wave functions to compute the expectation value involved in the Wigner function. To do so, we must be careful with the identification of the variables $\hat{\Phi}(p)$ and $\hat{\Pi}(p)$ with $\hat{x}$ and $\hat{p}$ of the HO. First, note that when we discretize the momentum, the commutation relation in Eq. (2.47) becomes

$$[\,\hat{\Phi}(p'),\hat{\Pi}(p)\,] = i\,2\pi\delta(p'-p) \rightarrow [\,\hat{\Phi}(p_{n'}),\hat{\Pi}(p_n)\,] = i\,L\,\delta_{n'n}\,, \tag{C.39}$$

where $\delta_{n',n}$ is the Kronecker delta. Clearly, this is not in the form of the quantum mechanical commutation relation $[\hat{x}_{n'},\hat{p}_n] = i\delta_{n'n}$. But it can be put in this form by redefining the field $\Phi(p)$ by $\overline{\Phi}(p) \rightarrow \Phi(p)/L$.

Therefore, implementing the discretization and using Eqs. (C.36)-(C.38), one can write Eq. (C.35) as:

$$\widetilde{W}^{(0)}_{\beta}[\Phi,\Pi] = \frac{1}{Z^{(0)}}\prod_{p}\widetilde{w}^{(0)}_{\beta}[\Phi_R(p),\Pi_R(p)]\times\widetilde{w}^{(0)}_{\beta}[\Phi_I(p),\Pi_I(p)]\,, \tag{C.40}$$

where $\widetilde{w}_{\beta}[\Phi_{R,I}(p),\Pi_{R,I}(p)]$ are the Wigner functions for just one momentum mode p, namely (to avoid clutter we omit the p dependence in the fields):

$$\begin{aligned}\widetilde{w}_{\beta}[\Phi_R,\Pi_R] &= \int_{-\infty}^{\infty} d\varphi_R\, e^{-\frac{i}{L}\Pi_R\,\varphi_R} \\ &\quad\times\left\langle \Phi_R+\frac{\varphi_R}{2}\middle| e^{-\frac{\beta}{2L}\left[\hat{\Pi}_R^2+(p^2+m^2)\hat{\Phi}_R^2\right]}\middle|\Phi_R-\frac{\varphi_R}{2}\right\rangle,\end{aligned} \tag{C.41}$$

and similarly for $\widetilde{w}_{\beta}[\Phi_I,\Pi_I]$. Next, we rewrite the operator in the second exponential in way that one use the known energy eigenfunctions of the HO. Specifically,

$$\begin{aligned}\hat{H} &= \frac{1}{2L}\hat{\Pi}_R^2+\frac{1}{2L}(p^2+m^2)\hat{\Phi}_R^2 \\ &= \frac{1}{2L}\hat{\Pi}_R^2+\frac{1}{2}(p^2+m^2)L\,\hat{\tilde{\Phi}}_R^2,\end{aligned} \tag{C.42}$$

so that L plays the role of the M and (p^2+m^2) plays the role of ω^2 in the HO Hamiltonian:

$$\hat{H}_{HO} = \frac{1}{2M}\hat{p}^2+\frac{1}{2}M\omega^2\hat{x}^2\,. \tag{C.43}$$

The eigenvalues of $\hat{H}_{HO}$ are $E_n = (n+1/2)\omega$ and the corresponding eigenstates are

$$\langle x|n\rangle = \psi_n(x) = \frac{1}{\sqrt{2^n n!}}\left(\frac{M\omega}{\pi}\right)^{1/4} H_n(\sqrt{M\omega}\,x)\, e^{-\frac{1}{2}M\omega x^2}\,, \tag{C.44}$$

where $H_n(x)$ are Hermite polynomials. Then, using the correspondence $M = L$ and $M\omega = E(p)L$, we can write for $\widetilde{w}_\beta[\Phi_R, \Pi_R]$:

$$\begin{aligned}
\widetilde{w}_\beta[\Phi_R,\Pi_R] &= \int_{-\infty}^{\infty} d\overline{\varphi}_R\, e^{-i\,\Pi_R\,\overline{\varphi}_R} \left\langle \overline{\Phi}_R + \frac{\overline{\varphi}_R}{2}\right| e^{-\frac{\beta}{L}\left[\hat{\Pi}_R^2 + (p^2+m^2)L\,\hat{\Phi}_R^2\right]} \left|\overline{\Phi}_R - \frac{\overline{\varphi}_R}{2}\right\rangle \\
&= \sum_n \frac{e^{-\beta\,(1/2+n)\,E}}{2^n n!}\left(\frac{EL}{\pi}\right)^{1/2} \int_{-\infty}^{\infty} d\overline{\varphi}_R\, e^{-i\,\Pi_R\,\overline{\varphi}_R} \\
&\quad \times H_n(X)\, H_n(Y)\, e^{-\frac{1}{2}\left(X^2+Y^2\right)}\,,
\end{aligned} \tag{C.45}$$

where we denoted $X = \sqrt{EL}\left(\overline{\Phi}_R + \overline{\varphi}_R/2\right)$ and $Y = \sqrt{EL}\left(\overline{\Phi}_R - \overline{\varphi}_R/2\right)$. We now use the result

$$\sum_n^{\infty} \frac{a^n}{n!} H_n(X) H_n(Y) = \frac{1}{\sqrt{1-4a^2}} \exp\left[\frac{4aXY - 4a^2(X^2+Y^2)}{1-4a^2}\right], \tag{C.46}$$

with $a = e^{-\beta E}/2$, which leads to

$$\begin{aligned}
\widetilde{w}_\beta[\Phi_R,\Pi_R] &= \frac{e^{-\frac{\beta E}{2}}}{\sqrt{1-4a^2}}\left(\frac{EL}{\pi}\right)^{1/2} \int_{-\infty}^{\infty} d\overline{\varphi}_R\, e^{-i\,\Pi_R\,\overline{\varphi}_R} \\
&\quad \times \exp\left[-\frac{1}{2}\left(X^2+Y^2\right) + \frac{4aXY - 4a^2(X^2+Y^2)}{1-4a^2}\right].
\end{aligned} \tag{C.47}$$

We write now the exponent of the last exponential in terms of $\overline{\Phi}$ and $\overline{\varphi}$:

$$\begin{aligned}
-\frac{X^2+Y^2}{2} + \frac{4aXY - 4a^2(X^2+Y^2)}{1-4a^2} &= -EL\left(\frac{1-2a}{1+2a}\,\overline{\Phi}^2 + \frac{1}{4}\,\frac{1+2a}{1-2a}\,\overline{\varphi}^2\right) \\
&= -EL\left[\tanh(\beta E/2)\,\overline{\Phi}^2 + \frac{1}{4\tanh(\beta E/2)}\,\overline{\varphi}^2\right].
\end{aligned} \tag{C.48}$$

The $\overline{\varphi}$ integral amounts to a Fourier transform of a Gaussian (Appendix A):

$$\int_{-\infty}^{\infty} d\overline{\varphi}\, e^{-i\,\Pi\,\overline{\varphi} - \frac{EL}{4\tanh(\beta E/2)}\,\overline{\varphi}^2} = \left[\frac{4\tanh(\beta E/2)}{EL}\right]^{1/2} e^{-\frac{\tanh(\beta E/2)}{EL}\,\Pi^2}. \tag{C.49}$$

Putting all together, we then obtain for $\widetilde{w}_\beta[\Phi_R, \Pi_R]$:

$$\begin{aligned}
\widetilde{w}_\beta[\Phi_R, \Pi_R] &= \frac{2\, e^{-\beta E/2}}{\sqrt{\tanh(\beta E/2)}}\, e^{-EL\left[\tanh(\beta E/2)\,\overline{\Phi}_R^2 + \frac{\tanh(\beta E/2)}{E^2L^2}\,\Pi_R^2\right]} \\
&= \frac{2\, e^{-\beta E/2}}{\sqrt{\tanh(\beta E/2)}}\, e^{-\frac{\tanh(\beta E/2)}{EL}\left(\Pi_R^2 + E^2L^2\,\overline{\Phi}_R^2\right)} \\
&= \frac{2\, e^{-\beta E/2}}{\sqrt{\tanh(\beta E/2)}}\, e^{-\frac{\beta}{L}\,\frac{2\tanh(\beta E/2)}{\beta E}\,\frac{1}{2}\left(\Pi_R^2 + E^2\,\Phi_R^2\right)} \\
&= \frac{2\, e^{-\beta E/2}}{\sqrt{\tanh(\beta E/2)}}\, e^{-\frac{\beta}{L}\,\tilde{\Delta}_\beta\,\frac{1}{2}\left(\Pi_R^2 + E^2\,\Phi_R^2\right)}\,, \qquad \text{(C.50)}
\end{aligned}$$

where

$$\tilde{\Delta}_\beta = \frac{2}{\beta E}\,\tanh(\beta E/2)\,. \qquad \text{(C.51)}$$

Finally, one can absorb the overall constant (w.r.t. to the fields) into Z in Eq. (C.40) and call this constant C, and write back the integrals in momentum from $-\infty$ to $+\infty$. One can then write the result for $\widetilde{W}_\beta^{(0)}[\Phi, \Pi]$ as

$$\begin{aligned}
\widetilde{W}_\beta^{(0)}[\Phi, \Pi] &= C\, e^{-\beta \int_{-\infty}^{\infty} \frac{dp}{2\pi}\,\tilde{\Delta}_\beta(p)\,\frac{1}{2}\left\{\Pi_R^2(p) + \Pi_I^2(p) + (p^2+m^2)\left[\Phi_R^2(p) + \Phi_I^2(p)\right]\right\}} \\
&= C\, e^{-\beta \int_{-\infty}^{\infty} \frac{dp}{2\pi}\,\tilde{\Delta}_\beta(p)\,\frac{1}{2}\left[\Pi^*(p)\Pi(p) + (p^2+m^2)\,\Phi^*(p)\Phi(p)\right]}\,, \qquad \text{(C.52)}
\end{aligned}$$

which is the desired result. Again, it is important to note that when this result is used in a path integration over fields $\Pi(p)$ and $\Phi(p)$, the momentum integral in the above expression must be restricted to the interval $p \in [0, \infty)$.

C.3.2 Proof of Normalization

We can fix the normalization of the Wigner functional by requiring a normalized density matrix, i.e. $\mathrm{Tr}\,\hat{\rho} = 1$. This leads to the condition:

$$\int D\Phi(p)\frac{D\Pi(p)}{2\pi}\tilde{W}_\beta(\Phi(p), \Pi(p)) = 1\,, \qquad \text{(C.53)}$$

using Eq. (3.65) for the Wigner functional in thermal equilibrium. We recall that $\Phi(p)$ and $\Pi(p)$ are complex field variables under the constraint $\Phi(-p) = \Phi^*(p)$ (same for Π) and so we need to restrict the integrals over p to positive values of p. We separate the fields into real and imaginary parts and discretize the momentum

integrals (restricting of course the sums to positive momenta):

$$\begin{aligned} 1 &= C\int \frac{D\Pi_R(p)}{2\pi}\,\exp\left[-\sum_{p>0}\frac{2\tanh(\frac{\beta E(p)}{2})}{E(p)L}\Pi_R^2(p)\right] \\ &\times\int \frac{D\Pi_I(p)}{2\pi}\exp\left[-\sum_{p>0}\frac{2\tanh(\frac{\beta E(p)}{2})}{E(p)L}\Pi_I^2(p)\right] \\ &\times\int D\Phi_R(p)\,\exp\left[-\sum_{p>0}\frac{2E(p)\tanh(\frac{\beta E(p)}{2})}{L}\Phi_R^2(p)\right] \\ &\times\int D\Phi_I(p)\,\exp\left[-\sum_{p>0}\frac{2E(p)\tanh(\frac{\beta E(p)}{2})}{L}\Phi_I^2(p)\right]. \end{aligned} \tag{C.54}$$

We see that we get four functional integrals (in Π_R, Π_I, Φ_R and Φ_I) similar in form to each other, up to a $1/2\pi$ factor; each integral means

$$\begin{aligned} \int D\phi(p)\,e^{-\sum_p f(p)\phi^2(p)} &= \prod_p^n\int_{-\infty}^{\infty} d\phi(p)\,e^{-f(p)\phi^2(p)} \\ &= \int_{-\infty}^{\infty} d\phi(p_1)\,e^{-f(p_1)\phi^2(p_1)}\int_{-\infty}^{\infty} d\phi(p_2)\,e^{-f(p_2)\phi^2(p_2)} \\ &\quad\cdots\int_{-\infty}^{\infty} d\phi(p_n)\,e^{-f(p_n)\phi^2(p_n)} \\ &= \sqrt{\frac{\pi}{f(p_1)}}\sqrt{\frac{\pi}{f(p_2)}}\cdots\sqrt{\frac{\pi}{f(p_n)}} = \prod_p^n\sqrt{\frac{\pi}{f(p)}}, \end{aligned} \tag{C.55}$$

where $\phi(p)$ stands for any of Π_R, Π_I, Φ_R and Φ_I. To simplify the notation, we make:

$$\begin{aligned} a(p) &= \frac{2\tanh\frac{\beta E(p)}{2}}{E(p)L}, \\ b(p) &= \frac{2E(p)\tanh\frac{\beta E(p)}{2}}{L}, \end{aligned} \tag{C.56}$$

and rewrite the integrals as

$$\begin{aligned} 1 &= C\int \frac{D\Pi_R(p)}{2\pi}\,\exp\left[-\sum_p a(p)\Pi_R^2(p)\right]\int \frac{D\Pi_I(p)}{2\pi}\exp\left[-\sum_p a(p)\Pi_I^2(p)\right] \\ &\quad\times\int D\Phi_R(p)\,\exp\left[-\sum_p b(p)\Phi_R^2(p)\right]\int D\Phi_I(p)\,\exp\left[-\sum_p b(p)\Phi_I^2(p)\right] \\ &= C\prod_p^n \frac{1}{2\pi}\sqrt{\frac{\pi}{a(p)}}\prod_p^n \frac{1}{2\pi}\sqrt{\frac{\pi}{a(p)}}\prod_p^n \sqrt{\frac{\pi}{b(p)}}\prod_p^n \sqrt{\frac{\pi}{b(p)}} \\ &= C\prod_p^n \frac{1}{4}\sqrt{\frac{1}{a^2(p)b^2(p)}}. \end{aligned} \tag{C.57}$$

Using our previous definitions for $a(p)$ and $b(p)$

$$1 = C\,L^{-2n}\prod_p^n \frac{1}{4}\sqrt{\frac{E^2(p)L^2}{4\tanh^2\frac{\beta E(p)}{2}}\,\frac{L^2}{4E^2(p)\tanh^2\frac{\beta E(p)}{2}}}, \tag{C.58}$$

and doing some algebra it is easy to show that

$$\begin{aligned} 1 &= C\,(2L)^{-2n}\prod_p \frac{L^2}{4\tanh^2\frac{\beta E(p)}{2}} = C\,(2L)^{-2n}\,\exp\left\{\ln\prod_p\left[\frac{1}{4\,\tanh^2\frac{\beta E(p)}{2}}\right]\right\} \\ &= C\,(2L)^{-2n}\,\exp\left\{\sum_{p>0}\ln\left[\frac{1}{4\,\tanh^2\frac{\beta E(p)}{2}}\right]\right\}. \end{aligned} \tag{C.59}$$

We now restore the continuous limit:

$$1 = C\,(2L)^{-2n}\,\exp\left\{-L\int_{-\infty}^{\infty}\frac{dp}{2\pi}\ln\left[2\tanh\frac{\beta E(p)}{2}\right]\right\}, \tag{C.60}$$

where we have changed the integration limits in the last step. One can see that isolating C we find

$$C = (2L)^{2n}\,\exp\left\{L\int_{-\infty}^{\infty}\frac{dp}{2\pi}\ln\left[2\tanh\frac{\beta E(p)}{2}\right]\right\}. \tag{C.61}$$

We note that the factor $(2L)^{2n}$ is temperature independent and can be absorbed in C (it could be absorbed in the normalization of integration measure also) i.e. we

could have defined

$$C' \equiv (2L)^{-2n} C = \exp\left\{ L \int_{-\infty}^{\infty} \frac{dp}{2\pi} \ln\left[2\tanh(\frac{\beta E(p)}{2}) \right] \right\}, \tag{C.62}$$

which is the result of Ref. [11].

C.3.3 Two Point Correlation Function

We insert Eq. (3.65) in Eq. (3.50) for $\mathcal{O}(\hat{\Phi}, \hat{\Pi}) = \hat{\Phi}^\dagger(p)\hat{\Phi}(p)$:

$$\begin{aligned}
\langle \hat{\Phi}^\dagger(p)\hat{\Phi}(p) \rangle &= \frac{1}{Z} \int D\Phi(p) \frac{D\Pi(p)}{2\pi} \, \Phi^*(p)\, \Phi(p)\, \widetilde{W}_\beta(\Phi(p), \Pi(p)) \\
&= \frac{C}{Z} \int D\Phi(p) \frac{D\Pi(p)}{2\pi} \, \Phi^*(p)\, \Phi(p) \\
&\quad \times \exp\left[-\frac{\beta}{2} \int_{-\infty}^{\infty} \frac{dp}{2\pi} \tilde{\Delta}_\beta(p) \left(\Pi^*(p)\Pi(p) + E^2(p)\Phi^*(p)\Phi(p) \right) \right],
\end{aligned} \tag{C.63}$$

In the same fashion as previous sections we separate the functional integrals in real and imaginary parts and discretize the momentum integrals inside the exponential

$$\begin{aligned}
\langle \hat{\Phi}^\dagger(p)\hat{\Phi}(p) \rangle &= \frac{C'}{Z} \int D\Phi_R(p) D\Phi_I(p) \left(\Phi_R^2(p) + \Phi_I^2(p) \right) \\
&\quad \times \exp\left[-\sum \frac{E(p) \tanh \frac{\beta E(p)}{2}}{L} \left(\Phi_R^2(p) + \Phi_I^2(p) \right) \right] \\
&\quad \times \int \frac{D\Pi_R(p)}{\pi} \frac{D\Pi_I(p)}{\pi} \exp\left[-\sum \frac{\tanh \frac{\beta E(p)}{2}}{E(p)L} \left(\Pi_R^2(p) + \Pi_I^2(p) \right) \right],
\end{aligned} \tag{C.64}$$

where we have changed to C' instead of C to absorb the $1/4$ and all irrelevant constants there will be. We can see that we have two terms to integrate, and they are equal in value. We already did the integrals in $\Pi(p)$ and in Φ in Section C.3.2. The integrals in $\Phi(p)$ with Φ^2 are a little bit trickier; we can make the substitution $a(p) = \frac{2\tanh(\frac{\beta E(p)}{2})}{E(p)L}$ and $b(p) = \frac{2E(p)\tanh(\frac{\beta E(p)}{2})}{L}$ again in the exponentials so that we

can write $\Phi^2_{R/I}(p) = -\frac{d}{db(p)}$ outside the integral. What we have is

$$\begin{aligned}
\langle\hat{\Phi}^\dagger(p)\hat{\Phi}(p)\rangle &= I_\phi I_{\phi\pi} + I_\phi I_{\phi\pi} \\
&= \frac{C'}{Z}\int D\Phi_R(p)\,\Phi^2_R(p)\,e^{-\sum b(p)\Phi^2_R(p)}\int D\Phi_I(p)\,e^{-\sum b(p)\Phi^2_I(p)} \\
&\quad\times\int\frac{D\Pi_R(p)}{\pi}\,e^{-\sum a(p)\Pi^2_R(p)}\frac{D\Pi_I(p)}{\pi}\,e^{-\sum a(p)\Pi^2_I(p)} \\
&\quad+\frac{C'}{Z}\int D\Phi_R(p)\,e^{-\sum b(p)\Phi^2_R(p)}\int D\Phi_I(p)\,\Phi^2_I(p)\,e^{-\sum b(p)\Phi^2_I(p)} \\
&\quad\times\int\frac{D\Pi_R(p)}{\pi}\,e^{-\sum a(p)\Pi^2_R(p)}\frac{D\Pi_I(p)}{\pi}\,e^{-\sum a(p)\Pi^2_I(p)}\,. \qquad \text{(C.65)}
\end{aligned}$$

We need to evaluate only one of these path integrals, i.e.

$$\langle\hat{\Phi}^\dagger(p)\hat{\Phi}(p)\rangle = 2I_\phi\,I_{\phi\Pi}\,, \qquad \text{(C.66)}$$

where $\phi = \Phi_R$ or $\phi = \Phi_I$. We start with I_ϕ:

$$\begin{aligned}
I_\phi &= \int D\phi(p)\,\phi^2(p)\,e^{-\sum b(p)\phi^2(p)} \\
&= \int_{-\infty}^{\infty} d\phi(p_1)\,e^{-b(p_1)\phi^2(p_1)}\;\cdots\;\left[-\frac{d}{db(p_i)}\int_{-\infty}^{\infty}d\phi(p_i)\,e^{-b(p_i)\phi^2(p_i)}\right] \\
&\quad\cdots\int_{-\infty}^{\infty}d\phi(p_n)\,e^{-b(p_n)\phi^2(p_n)} \\
&= \sqrt{\frac{\pi}{b(p_1)}}\;\cdots\;\left[-\frac{d}{db(p_i)}\sqrt{\frac{\pi}{b(p_i)}}\right]\;\cdots\;\sqrt{\frac{\pi}{b(p_n)}} \\
&= \sqrt{\frac{\pi}{b(p_1)}}\;\cdots\;\frac{1}{2b(p_i)}\sqrt{\frac{\pi}{b(p_i)}}\;\cdots\;\sqrt{\frac{\pi}{b(p_n)}} = \frac{1}{2b(p)}\prod_p\sqrt{\frac{\pi}{b(p)}}\,. \qquad \text{(C.67)}
\end{aligned}$$

Next, we evaluate $I_{\phi\Pi}$:

$$\begin{aligned}
I_{\phi\Pi} &= \frac{C'}{Z}\int D\Phi_I(p)\,e^{-\sum b(p)\Phi^2_I(p)}\int\frac{D\Pi_R(p)}{\pi}\,e^{-\sum a(p)\Pi^2_R(p)} \\
&\quad\times\int\frac{D\Pi_I(p)}{\pi}\,e^{-\sum a(p)\Pi^2_I(p)} \\
&= \frac{C'}{Z}\prod_p\frac{1}{\pi^2}\sqrt{\frac{\pi^3}{a^2(p)b(p)}}\,. \qquad \text{(C.68)}
\end{aligned}$$

One then obtains for the two point correlation function:

$$\begin{aligned}\langle\hat{\Phi}^{\dagger}(p)\hat{\Phi}(p)\rangle &= \frac{2C'}{Z}\frac{1}{2b(p)}\prod_{p}^{n}\sqrt{\frac{\pi}{b(p)}}\prod_{p}\frac{1}{\pi^2}\sqrt{\frac{\pi^3}{a^2(p)b(p)}} \\ &= \frac{C'}{Z}\frac{1}{b(p)}\prod_{p}^{n}\sqrt{\frac{1}{a^2(p)b^2(p)}}\,. \end{aligned} \tag{C.69}$$

Making use of Z:

$$Z = C'\prod_{p}^{n}\sqrt{\frac{1}{a^2(p)b^2(p)}}\,, \tag{C.70}$$

we arrive at

$$\langle\hat{\Phi}^{\dagger}(p)\hat{\Phi}(p)\rangle = \frac{1}{b(p)} = \frac{L}{2E(p)\tanh\frac{\beta E(p)}{2}}\,. \tag{C.71}$$

The $\langle\hat{\Pi}^{\dagger}(p)\hat{\Pi}(p)\rangle$ is analogous; following the same steps but with Π instead, one obtains

$$\langle\hat{\Pi}^{\dagger}(p)\hat{\Pi}(p)\rangle = \frac{E(p)L}{2\tanh\frac{\beta E(p)}{2}}\,. \tag{C.72}$$

Appendix D

Gibbs Variational Principle

The Gibbs variational principle makes two statements. The first statement is that one obtains the equilibrium density matrix $\hat{\rho}_{eq}$ of the canonical ensemble for a given Hamiltonian $\hat{H}$:

$$\hat{\rho}_{eq} = \frac{1}{Z_{eq}} e^{-\beta \hat{H}} \qquad \text{with} \qquad Z_{eq} = \operatorname{Tr} e^{-\beta \hat{H}} \tag{D.1}$$

by minimizing the functional

$$\psi(\hat{\rho}) = \operatorname{Tr}(\hat{H}\,\hat{\rho}) + \frac{1}{\beta} \operatorname{Tr}(\hat{\rho}\,\ln \hat{\rho})\,, \tag{D.2}$$

with respect to $\hat{\rho}$ under the assumption that $\hat{\rho}$ is a positive density matrix normalized to unity:

$$\operatorname{Tr} \hat{\rho} = 1\,. \tag{D.3}$$

The second statement is that the Helmholtz free energy F is given by

$$F = -\frac{1}{\beta} \ln Z_{eq} = \psi(\hat{\rho}_{eq})\,. \tag{D.4}$$

We follow Ref. [65] to prove the two statements. Let's evaluate the first $\delta\psi$ and second $\delta^2\psi$ variations of $\psi(\hat{\rho})$:

$$\delta\psi = \operatorname{Tr}(\hat{H}\delta\hat{\rho}) + \frac{1}{\beta} \operatorname{Tr}\, \delta\hat{\rho} \ln \hat{\rho} + \delta\hat{\rho} = \operatorname{Tr}\left[\left(\hat{H} + \frac{1}{\beta}(1 + \ln \hat{\rho})\right)\delta\hat{\rho}\right]\,, \tag{D.5}$$

$$\delta^2\psi = \operatorname{Tr}\left[\left(0 + \frac{1}{\beta}(0 + \hat{\rho}^{-1}\,\delta\hat{\rho})\right)\delta\hat{\rho}\right] = \frac{1}{\beta} \operatorname{Tr}\left[\hat{\rho}^{-1}\,(\delta\rho)^2\right]\,. \tag{D.6}$$

Since $\delta^2\psi > 0$ (because $\hat{\rho}$ is positive), we conclude that $\psi(\hat{\rho})$ is a convex function and so $\delta\psi = 0$ is a minimum. Next, we vary $\hat{\rho}$ under the normalization constraint

in Eq. (D.3) using a Lagrange multiplier λ:

$$0 = \delta\psi + \lambda\,\delta(\mathrm{Tr}\,\hat{\rho}) = \mathrm{Tr}\,\left[\left(\hat{H} + \frac{1}{\beta}(1+\ln\hat{\rho}) + \lambda\right)\delta\hat{\rho}\right]. \tag{D.7}$$

Since $\delta\hat{\rho}$ is arbitrary:

$$\hat{H} + \frac{1}{\beta}(1+\ln\hat{\rho}) + \lambda = 0\,, \tag{D.8}$$

and we conclude that

$$\hat{\rho} = e^{-(1+\beta\lambda)}e^{-\beta\hat{H}}\,. \tag{D.9}$$

One determines λ using the normalization condition:

$$1 = \mathrm{Tr}\;\hat{\rho} = \mathrm{Tr}\;\left[e^{-(1+\beta\lambda)}e^{-\beta\hat{H}}\right] = e^{-(1+\beta\lambda)}\;\mathrm{Tr}\;e^{-\beta\hat{H}}\,. \tag{D.10}$$

Substituting this result in Eq. (D.9) proves the first statement. Now, using this result in Eq. (D.2) proves the second statement:

$$\begin{aligned}\psi(\hat{\rho}_{eq}) &= \mathrm{Tr}\;\left[\hat{H}\frac{e^{-\beta\hat{H}}}{\mathrm{Tr}\;e^{-\beta\hat{H}}}\right] + \frac{1}{\beta}\;\mathrm{Tr}\;\left[\frac{e^{-\beta\hat{H}}}{\mathrm{Tr}\;e^{-\beta\hat{H}}}\ln\left(\frac{e^{-\beta\hat{H}}}{\mathrm{Tr}\;e^{-\beta\hat{H}}}\right)\right] \\ &= -\frac{1}{\beta}\ln\left(\mathrm{Tr}\;e^{-\beta\hat{H}}\right).\end{aligned} \tag{D.11}$$

We use the Gibbs variational principle as follows. Let $\hat{\rho}$ be the normalized equilibrium density matrix corresponding to a Hamiltonian $\hat{H}$ and $\hat{\rho}_0$ a normalized equilibrium density matrix corresponding to a Hamiltonian $\hat{H}_0$, namely:

$$\hat{\rho} = \frac{1}{Z}\,e^{-\beta\hat{H}} \qquad \text{with} \qquad Z = \mathrm{Tr}\,e^{-\beta\hat{H}}\,, \tag{D.12}$$

and

$$\hat{\rho}_0 = \frac{1}{Z_0}\,e^{-\beta\hat{H}_0} \qquad \text{with} \qquad Z_0 = \mathrm{Tr}\,e^{-\beta\hat{H}_0}\,. \tag{D.13}$$

The Gibbs variational principle states that

$$F(\hat{\rho}) = \mathrm{Tr}(\hat{H}\hat{\rho}) + \frac{1}{\beta}\,\mathrm{Tr}(\hat{\rho}\ln\hat{\rho}) \leq \mathrm{Tr}(\hat{H}\hat{\rho}_0) + \frac{1}{\beta}\,\mathrm{Tr}(\hat{\rho}_0\ln\hat{\rho}_0)\,. \tag{D.14}$$

Now, if $\hat{H} = \hat{H}_0 + \hat{H}_1$, this is equivalent to

$$\begin{aligned} F(\hat{\rho}) &\leq \mathrm{Tr}(\hat{H}_0\hat{\rho}_0) + \mathrm{Tr}(\hat{H}_1\hat{\rho}_0) + \frac{1}{\beta}\,\mathrm{Tr}(\hat{\rho}_0 \ln \hat{\rho}_0) \\ &= \mathrm{Tr}(\hat{H}_0\hat{\rho}_0) + \mathrm{Tr}(\hat{H}_1\hat{\rho}_0) - \mathrm{Tr}(\hat{H}_0\hat{\rho}_0) + F(\hat{\rho}_0) \\ &= F(\hat{\rho}_0) + \mathrm{Tr}(\hat{H}_1\hat{\rho}_0)\,, \end{aligned} \tag{D.15}$$

where we used that

$$F(\hat{\rho}_0) = -\frac{1}{\beta}\ln Z_0\,. \tag{D.16}$$

Suppose that $\hat{H}_0$ depends on some undetermined parameters $g_1, \ldots, g_n$, i.e. $\hat{H}_0 = \hat{H}_0(g_1, \ldots, g_n)$; thereby $\hat{\rho}_0 = \hat{\rho}_0(g_1, \ldots, g_n)$. One can determine the parameters $g_1, \ldots, g_n$ by treating them as variational trial parameters in the Gibbs variational principle, namely:

$$F(\hat{\rho}) \leq F(\hat{\rho}_0) + \mathrm{Tr}(\hat{H}_1\hat{\rho}_0) \equiv F_{var}(g_1, \ldots, g_n), \tag{D.17}$$

with

$$\frac{\partial F_{var}(g_1, \ldots, g_n)}{\partial g_i} = 0 \qquad \text{for} \qquad i = 1, \ldots, n\,. \tag{D.18}$$

In our case, $\hat{H}_0 = \hat{H}_q$ and $\hat{H}_1 = H'(q \in \mathcal{S}) + H''(q \notin \mathcal{S})$, and the $g(k, q)$ are the trial parameters.

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