Quantum kinetic theory of a Bose-Einstein gas confined in a lattice

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We extend our earlier work on the nonequilibrium dynamics of a Bose-Einstein condensate initially loaded into a one-dimensional optical lattice. From the two-particle-irreducible (2PI) closed-time-path (CTP) effective action for the Bose-Hubbard Hamiltonian we derive causal equations of motion that treat mean-field effects and quantum fluctuations on an equal footing. We demonstrate that these equations reproduce well-known limits when simplifying approximations are introduced. For example, when the system dynamics admits two-time separation, we obtain the Kadanoff-Baym equations of quantum kinetic theory, and in the weakly interacting limit, we show that the local equilibrium solutions of our equations reproduce the second-order corrections to the self-energy of the type originally derived by Beliaev. The derivation of quantum kinetic equations from the 2PI-CTP effective action not only checks the viability of the formalism but also shows it to be a tractable framework for going beyond standard Boltzmann equations of motion.

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I. INTRODUCTION

In many respects, the dynamics of cold atoms in optical lattices resembles that of electrons in crystals. Cold-atom systems exhibit many favorable attributes for studying quantum many-body dynamics such as the absence of defects in the optical lattice and the high degree of experimental control over all relevant parameters [1,2]. In particular, by varying the depth of the optical lattice, the superfluid-insulator phase transition can be induced. For weakly confining optical lattices, the system has macroscopic quantum coherence, and interesting matter-wave interference phenomena induced by the periodicity of the lattice have been demonstrated in experiments [3–6]. For tightly confining lattices, the matter-wave coherence is lost, and the system undergoes a transition to the Mott-insulator phase [7]. This regime has become also experimentally accessible [8–10]. Outside the weakly interacting regime, standard mean-field techniques are inapplicable to describe the evolution of the system and alternative methods are required [11].

We previously adopted a functional effective-action approach capable of dealing with nonequilibrium situations that require a treatment beyond mean-field theory ([12], hereafter I). That work applied the closed-time-path (CTP) functional formalism [13] and the two-particle-irreducible (2PI) effective action [14] to the Bose-Hubbard Hamiltonian, and derived equations of motion. That method enabled us to go beyond the Hartree-Fock-Bogoliubov (HFB) approximation [15–17] and to incorporate nonlinear and non-Markovian aspects of quantum dynamics, which underlie dissipation and fluctuation phenomena. In its pristine form the 2PI-CTP equations of motion for the mean field and the two-point correlation function are complicated nonlocal nonlinear equations, which defy even numerical solutions for realistic experimental systems with many lattice sites. It is obvious that to get more physical insight we need ways to simplify this full theory.

In the present paper, we pursue such simplifications by deriving quantum kinetic theory from the 2PI-CTP formalism [18,19]. Towards this goal, we ask the question when quantum kinetic theory is a reasonably attainable limit of the more complete theory based on the 2PI-CTP effective action. Physically, a kinetic theory regime exists when the system dynamics has a clear separation of two time (or length) scales, one pertaining to the macroscopic scale describing the kinetic motion such as the mean free time and the other to the microscopic scale such as the duration of collision events. Alternatively, when perturbations induce disturbances of wavelength longer than the thermal wavelengths and frequencies much lower than characteristic excitation frequencies, standard kinetic theories may give a reasonable description of the system's dynamics. This is the case for weakly interacting gases confined by a slowly varying external potential. For quantum systems, when the quantum features of the many-body system act effectively only on the microscopic scale (e.g., when one can use a quasiparticle type of approximation), quantum kinetic theory can provide an adequate description. It fails when such a two-time separation does not exist, such as in strongly correlated systems or systems with macroscopic quantum coherence.[1]

Recent independent work along these lines [20] has derived kinetic equations for the case of an unconfined Bose-

[1]We have in mind systems whose quantum coherence or correlation or entanglement extends to macroscopic dimensions. Examples are coherence tunneling phenomena [43], quantum properties of microelectromechanical systems [44,45], and, of course, Bose-Einstein condensation (BEC), which certainly has macroscopic quantum coherence. The impossibility of a two-time separation refers only to the condensate state alone. The interaction between the condensate and the non-condensate atoms can under general conditions allow a two-time separation and a kinetic theory description, as is the topic of our present discussion and much prior work.

Einstein gas, starting from the 2PI effective action of a relativistic scalar field. Earlier work addressing this problem in quantum field theory can be found in Refs. [21–27]. There exists an extensive literature on quantum kinetic theory, much of which addresses the dynamics of a BEC interacting with a noncondensate component of the gas [15,28–42]. Work particularly relevant to our present discussions includes [15,28–34].

The organization of this paper with a brief of our findings is as follows. In Sec. II we summarize our prior results for the HFB and second-order equations of motion [12] and express them with lightened notation in a more compact form. In Sec. III we discuss how a quantum kinetic theory can be derived from a quantum theory of interacting particles. We first discuss this issue under more general conditions, where a two-time separation may not exist. A kinetic theory is obtained from the full hierarchy of correlation functions by truncation of higher-order correlations and the imposition of causal factorizable conditions. We use the *n*PI-effective action to illustrate this conceptual framework. In Sec. IV we focus on situations where there is a two-time separation in the system dynamics. We delineate the physical conditions and show the procedures in deriving quantum kinetic equations from the 2PI-CTP equations of motion. Then we introduce further simplifications and discuss how to derive the familiar Boltzmann equations. In Sec. V we study how these kinetic equations admit, as a special yet important case, equilibrium solutions. We show that under the Popov approximation the second-order 2PI equations yield to the same second-order damping rates originally obtained in Beliaev's pioneered work [46] but with a modified effective mass due to the presence of the lattice. In Sec. VI we conclude with a few general remarks.

II. 2PI-CTP EFFECTIVE ACTION FOR THE BOSE-HUBBARD HAMILTONIAN

Here we summarize the structure of this method and collect the useful equations obtained from our earlier investigation [12].

A. Bose-Hubbard Hamiltonian

The one-dimensional Bose-Hubbard Hamiltonian is given by

$$\hat{H} = -J\sum_i (\hat{a}_i^\dagger \hat{a}_{i+1} + \hat{a}_{i+1}^\dagger \hat{a}_i) + \sum_i V_i \hat{n}_i + \frac{U}{2}\sum_i \hat{n}_i(\hat{n}_i - 1), \tag{1}$$

where $\hat{a}_i$ and $\hat{a}_i^\dagger$ (called $\hat{\Phi}_i, \hat{\Phi}_i^\dagger$ in paper I) are the bosonic operators that annihilate and create an atom on the site i and $\hat{n}_i \equiv \hat{a}_i^\dagger \hat{a}_i$ is the number operator at site i. The parameter U denotes the strength of the on-site repulsion of two atoms on the site i, and $J/\hbar$ denotes the hopping rate between adjacent sites. Next-to-nearest-neighbor tunneling matrix elements are typically two orders of magnitude smaller than the nearest-neighbor ones, and to a good approximation they can be neglected. The parameter V_i (called ϵ_i in paper I) denotes the energy offset of each lattice site due to an additional external potential that might be present (such as a magnetic trap). In contrast to the previous paper, where we set $V_i(t)=0$, here we allow the presence of an external potential. We will assume that V_i is a slowly varying function in position and time and treat it as an external perturbation. The Bose-Hubbard Hamiltonian should be an appropriate model [47] when the loading process produces atoms in the lowest vibrational state of each well, with a chemical potential smaller than the energy separation to the first vibrationally excited state.

We denote the mean field or the expectation value of the field operator by $\langle \hat{a}_i(t)\rangle = z_i(t)$ [called $\phi_i^a(t)$ in paper I] and the fluctuation field by $\hat{\varphi}_i(t) = \hat{a}_i(t) - z_i(t)$. Physically, $|z_i(t)|^2$ is related but not necessarily equal to the condensate population at site i. It cannot be just equated to the condensate because, in general ($V_i \neq 0$), it may not be an eigenfunction of the one-body density matrix [40,48].

In paper I we developed an index notation for the field operators and the two-point functions. This notation facilitated us the derivation of the 2PI-CTP equations of motion. Here, instead, to lighten the notation and to connect it to a more commonly use set of symbols, we introduce a matrix notation for the physical quantities:

$$\mathbf{z}(t_i) = \begin{pmatrix} \langle \hat{a}_i(t)\rangle \\ \langle \hat{a}_i^\dagger(t)\rangle \end{pmatrix} = \begin{pmatrix} z_i(t) \\ z_i^*(t) \end{pmatrix}, \tag{2}$$

$$iH(t_i, t_j') \equiv \begin{pmatrix} z_i(t) z_j^*(t') & z_i(t) z_j^*(t') \\ z_i^*(t) z_j^*(t') & z_i^*(t) z_j(t') \end{pmatrix}, \tag{3}$$

$$\mathrm{i}g(t_i, t_j') \equiv \begin{pmatrix} \langle T_C \hat{\varphi}_i(t) \hat{\varphi}_j^\dagger(t')\rangle & \langle T_C \hat{\varphi}_i(t) \hat{\varphi}_j(t')\rangle \\ \langle T_C \hat{\varphi}_i^\dagger(t) \hat{\varphi}_j^\dagger(t')\rangle & \langle T_C \hat{\varphi}_i^\dagger(t) \hat{\varphi}_j(t')\rangle \end{pmatrix}, \tag{4}$$

where the brackets denote taking the expectation value with respect to the density matrix and T_C denotes time ordering along a contour C in the complex plane. The notation t_i means that the function must be evaluated at the time t and at the lattice site i. Sometimes we will use this notation to shorten the equations.

The classical action associated with the Bose-Hubbard Hamiltonian is given in terms of the complex fields $z(t_i)$ and $z_i^*(t)$ by

$$S[\mathbf{z}] = \mathrm{i}\hbar \int_C dt \sum_i z_i^* \partial_t z_i + J \int_C dt \sum_i (z_i^* z_{i+1} + z_i z_{i+1}^*) - \int_C dt \sum_i V_i z_i^* z_i - \int_C dt \sum_i \frac{U}{2} z_i^* z_i^* z_i z_i, \tag{5}$$

where $\int_C$ denotes a contour integral along the C which we will specify later.

All correlation functions of the quantum theory can be obtained from the 2PI effective action $\Gamma[\mathbf{z}, g]$. In Ref. [12] we showed $\Gamma[\mathbf{z}, g]$ is given by

$$\Gamma[\mathbf{z},g] = S[\mathbf{z}] + \frac{i\hbar}{2}\mathrm{Tr}(\ln g^{-1}) + \frac{i\hbar}{2}\mathrm{Tr}(D_c^{-1}[\mathbf{z}]g) + \hbar\Gamma_2[\mathbf{z},g] + \mathrm{const.} \quad (6)$$

In Eq. (6) the symbol "Tr" denotes taking the trace over the 2×2 matrices and over both spatial and temporal degrees of freedom. D_c^{-1} is the classical inverse propagator defined as

$$D_c^{-1}(t_i,t_j') = D_0^{-1}(t_i,t_j') + D_{int}^{-1}(t_i,t_j'), \quad (7)$$

$$D_0^{-1}(t_i,t_j') = [i\delta_{ij}\sigma_z\partial_t + J(\delta_{i+1j} + \delta_{i-1j})]\delta(t-t') - \delta_{ij}V_i\delta(t-t'), \quad (8)$$

$$D_{int}^{-1}(t_i,t_j') = -\frac{iU}{2}\{2H(t_i,t_i') + I\mathrm{Tr}[H(t_i,t_i')]\}\delta_{ij}\delta(t-t'), \quad (9)$$

where D_0^{-1} is the inverse free-particle propagator. In this work we will not use the Einstein convention over repeated indexes unless specified. The symbol "Tr" denotes taking the trace over the 2×2 matrices, I is the 2×2 identity matrix, and σ_z is the z Pauli matrix:

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad (10)$$

$\Gamma_2[\mathbf{z},g]$ consists of all two-particle-irreducible vacuum graphs in the theory (the diagrams that do not become disconnected by cutting two propagator lines) with propagators set equal to g and vertices determined by the interaction terms in $S[\mathbf{z}+\varphi]$ which are cubic or higher order in the fluctuation field φ.

The dynamical equations of motion for the mean field $\mathbf{z}$ and the propagators g are found by minimizing the effective action: $\delta\Gamma[\mathbf{z},g]/\delta\mathbf{z}=0$ and $\delta\Gamma[\mathbf{z},g]/\delta g=0$. This procedure leads to the following equations of motion:

$$i\hbar\sigma_z\partial_t\mathbf{z}(t_i) = -J[\mathbf{z}(t_{i+1}) + \mathbf{z}(t_{i-1})] + V_i\mathbf{z}(t_i) + i\frac{U}{2}\{\mathrm{Tr}[H(t_i,t_i) + g(t_i,t_i)]\mathbf{z}(t_i) + 2g(t_i,t_i)\mathbf{z}(t_i)\} - \frac{\delta\Gamma_2[\mathbf{z},g]}{\delta\mathbf{z}(t_i)} \quad (11)$$

and

$$g^{-1}(t_i,t_j') = D_0^{-1}(t_i,t_j') + D_{int}^{-1}(t_i,t_j') - 2i\frac{\delta\Gamma_2[\mathbf{z},g]}{\delta g(t_i,t_j')}. \quad (12)$$

B. HFB and full second-order equations of motion

Various approximations for the full 2PI effective action can be obtained by truncating the diagrammatic expansion for Γ. The ones relevant for this paper are the *HFB approximation* and the *full second-order approximation*. The HFB approximation corresponds to a truncation of Γ retaining only the two-particle-irreducible diagram first order in U: $\Gamma_2=\Gamma_2^{(1)}[g]$. The full second-order approximation corresponds to a truncation retaining also the two-particle-irreducible diagrams second order in U: $\Gamma_2[\mathbf{z},g]=\Gamma_2^{(1)}[g]+\Gamma_2^{(2)}[\mathbf{z},g]$. Even though only terms up to second order in U are retained, by solving the equations for the propagators self-consistently one goes beyond the second-order truncation. We refer the interested reader to paper I for a detail explanation of these two approximations.

We now introduce the condensate and the two-point-function self-energies, defined as

$$\sum_k \int_C dt'' S^{HFB}(t_i,t_k'')H(t_k'',t_j') \equiv i\frac{U}{2}(\mathrm{Tr}[H(t_i,t_i) + g(t_i,t_i)]I + 2g(t_i,t_i))H(t_i,t_j), \quad (13)$$

$$\sum_k \int_C dt'' S(t_i,t_k'')H(t_k'',t_j') \equiv -\frac{\delta\Gamma_2^{(2)}[\mathbf{z},g]}{\delta\mathbf{z}(t_i)}\mathbf{z}^\dagger(t_j), \quad (14)$$

$$\Sigma^{HFB}(t_i,t_j') \equiv -D_{int}^{-1}(t_i,t_j') + 2i\frac{\delta\Gamma_2^{(1)}[\mathbf{z},g]}{\delta g(t_i,t_j')}, \quad (15)$$

$$\Sigma(t_i,t_j') \equiv 2i\frac{\delta\Gamma_2^{(2)}[\mathbf{z},g]}{\delta g(t_i,t_j')}. \quad (16)$$

Using these definitions, the equations of motion derived from the 2PI-CTP effective action [Eqs. (11) and (12)] can be rewritten in an integral form. The different terms in the equations can be grouped as the single-particle, the HFB, and the second-order contributions, as follows:

$$\sum_k \int_C dt''[D_0^{-1}(t_i,t_k'') - S^{HFB}(t_i,t_k'')]H(t_k'',t_j') = \sum_k \int_C dt'' S(t_i,t_k'')H(t_k'',t_j'), \quad (17)$$

$$\sum_k \int_C dt''[D_0^{-1}(t_i,t_k'') - \Sigma^{HFB}(t_i,t_k'')]g(t_k'',t_j') = \sum_k \int_C dt''\Sigma(t_i,t_k'')g(t_k'',t_j') + \delta_{ij}\delta_C(t-t'). \quad (18)$$

The expressions for the the HFB and second-order self-energies in terms of H and g are explicitly written in the Appendix.

C. Schwinger-Keldysh (CTP) contour

In order to describe the nonequilibrium dynamics we specify the contour of integration C to be the Schwinger-Keldysh contour [13] along the real-time axis or *closed-time-path* contour. The basic idea of the CTP formalism is to take a diagonal matrix element of a system at a given time t_0 and insert a complete set of states into this matrix element at the later time t. In this way one can be expressed the matrix element as a product of transition matrix elements from t_0 to t and the time-reverse (complex conjugate) matrix element from t to t_0. The time order in the time path from t_0 to t (which we denote by C^+) should be taken forward in time but backwards along the path from t to t_0 (which we denote by C^-).

Using the CTP contour, the two-point functions and self-energies are decomposed as

$$g(t_i,t_j') = \theta_{ctp}(t,t')g^{>}(t_i,t_j') + \theta_{ctp}(t',t)g^{<}(t_i,t_j'), \quad (19)$$

$$S(t_i,t_j') = \theta_{ctp}(t,t')S^{>}(t_i,t_j') + \theta_{ctp}(t',t)S^{<}(t_i,t_j'), \quad (20)$$

$$\Sigma(t_i,t_j') = \theta_{ctp}(t,t')\Sigma^{>}(t_i,t_j') + \theta_{ctp}(t',t)\Sigma^{<}(t_i,t_j'), \quad (21)$$

where $\theta_{ctp}(t,t')$ is the CTP complex-contour-ordered theta function defined as

$$\theta_{ctp}(t,t') = \begin{cases} \theta(t,t') \text{ for } t \text{ and } t' \text{ both on } C^+, \\ \theta(t',t) \text{ for } t \text{ and } t' \text{ both on } C^-, \\ 1 \text{ for } t \text{ on } C^- \text{ and } t' \text{ on } C^+, \\ 0 \text{ for } t \text{ on } C^+ \text{ and } t' \text{ on } C^-, \end{cases}$$

with $\theta(t,t')$ the step function. The propagators $g^{(\gtrless)}$ are given by

$$ig^{>}(t_i,t_j') \equiv \begin{pmatrix} \varsigma_{ij}(t,t') & m_{ij}(t,t') \\ m_{ji}^*(t',t) & \rho_{ji}(t',t) \end{pmatrix}, \quad (22)$$

$$ig^{<}(t_i,t_j') \equiv \begin{pmatrix} \rho_{ij}(t,t') & m_{ji}(t',t) \\ m_{ij}^*(t,t') & \varsigma_{ji}(t',t) \end{pmatrix}, \quad (23)$$

with

$$\varsigma_{ij}(t,t') \equiv \langle \hat{\varphi}_i(t)\hat{\varphi}_j^{\dagger}(t')\rangle \quad (24)$$

$$\rho_{ij}(t,t')) \equiv \langle \hat{\varphi}_j^{\dagger}(t')\hat{\varphi}_i(t)\rangle \quad (25)$$

$$m_{ij}(t,t') \equiv \langle \hat{\varphi}_i(t)\hat{\varphi}_j(t')\rangle. \quad (26)$$

At equal times, the quantities ς_{ij} and ρ_{ij} are related by the bosonic commutation relations. The explicit expression for the second-order self-energies $S^{(\gtrless)}$ and $\Sigma^{(\gtrless)}$, in terms of $g^{(\gtrless)}$ and their matrix components, can be found in the Appendix.

In paper I, we used the CTP contour of integration (which is also usually called "in-in" contour) to evaluate the *second-order contribution*. The use of the CTP formalism was important there, because it provided the technical means to formulate our initial-value problem in a completely causal manner, removing the Feynman boundary conditions on the Green's function used in the conventional "in-out" formalism. In this work we are more interested in deriving kinetic equations which are especially devised to study relaxation of systems close to equilibrium. With this purpose in mind, as done by Kadanoff and Baym [18,19], it is better to set the initial conditions in the far past. We follow them hereafter and use the CTP contour, but instead of setting the initial time to zero, as was done in paper I, we choose it to be $-\infty$. The equations of motion we obtain in this way agree with the equations of motion [18,19] and are given by

$$\sum_k \int_{-\infty}^{\infty} dt''[D_0^{-1}(t_i,t_k'') - S^{HFB}(t_i,t_k'')]H(t_k'',t_j') - \int_{-\infty}^{t} dt''\gamma(t_i,t_k'')H(t_k'',t_j') = 0, \quad (27)$$

$$\sum_k \int_{-\infty}^{\infty} dt''H(t_i,t_k'')[D_0^{-1}(t_k'',t_j') - S^{HFB}(t_k'',t_j')] + \int_{-\infty}^{t'} dt''H(t_i,t_k'')\gamma(t_k'',t_j') = 0, \quad (28)$$

$$\sum_k \int_{-\infty}^{\infty} dt''[D_0^{-1}(t_i,t_k'') - \Sigma^{HFB}(t_i,t_k'')]g^{(\gtrless)}(t_k'',t_j') = \sum_k \int_{-\infty}^{t} dt''\Gamma(t_i,t_k'')g^{(\gtrless)}(t_k'',t_j') - \sum_k \int_{-\infty}^{t'} dt''\Sigma^{(\gtrless)}(t_i,t_k'')A(t_k'',t_j'), \quad (29)$$

$$\sum_k \int_{-\infty}^{\infty} dt''g^{(\gtrless)}(t_i,t_k'')[D_0^{-1}(t_k'',t_j') - \Sigma^{HFB}(t_k'',t_j')] = \sum_k \int_{-\infty}^{t} dt''A(t_i,t_k'')\Sigma^{(\gtrless)}(t_k'',t_j') - \sum_k \int_{-\infty}^{t'} dt''g^{(\gtrless)}(t_i,t_k'')\Gamma(t_k'',t_j'). \quad (30)$$

In the above equations, Eq. (28) is the Hermitian conjugate of Eq. (27), Eq. (30) is the Hermitian conjugate of Eq. (29), and we have introduced the spectral functions

$$\gamma(t_i,t_j') \equiv S^{>}(t_i,t_j') - S^{<}(t_i,t_j'), \quad (31)$$

$$\Gamma(t_i,t_j'') \equiv \Sigma^{>}(t_i,t_j'') - \Sigma^{<}(t_i,t_j''), \quad (32)$$

$$A(t_i,t_j'') \equiv g^{>}(t_i,t_j'') - g^{<}(t_i,t_j''). \quad (33)$$

Notice that $A(t_i,t_j'')$, $\Gamma(t_i,t_j'')$, and $\gamma(t_i,t_j')$ are just the spectral functions defined in paper I [Eq. (136)] multiplied by a minus sign. In paper I we denoted these by a superscript (ρ). Here, for ease of comparisons with the literature, we have changed to the notation of Kadanoff and Baym [18]: γ, Γ, and A. We will show later that γ and Γ contain information about the condensate and noncondensate particle decay rates, respectively.

In Refs. [30,32] the authors used these equations as the starting point of a quantum kinetic theory before applying the Markovian approximation. It is important to mention that in contrast to other self-energy approximations that may lead to equations of motion that do not satisfy conservation laws, the 2PI effective action formalism is a "Φ-derivable" [49,50] approximation and therefore all the equations of motion derived from it are guaranteed to be conserving. Moreover, as we showed in paper I, a truncation up to second order in the interaction strength is not appropriate to describe far-from-equilibrium dynamics outside the weak-coupling regime. Away from the weak-coupling regime, the 2PI effective action can be a powerful tool. For example, a $1/\mathcal{N}$ expansion of the 2PI effective action has been shown to provide a practicable controlled nonperturbative description of far-from equilibrium dynamics [27]. In the large-$\mathcal{N}$ expansion the

field is modeled by $\mathcal{N}$ fields and the quantum field generating functional is expanded in powers of $1/\mathcal{N}$. In this sense the method is a controlled expansion in a small parameter, but unlike perturbation theory in the coupling constant U, the large-$\mathcal{N}$ expansion corresponds to an expansion of the theory about a strong quasiclassical field and does not have the small-coupling restriction.

III. FROM QUANTUM THEORY OF INTERACTING PARTICLES TO QUANTUM KINETIC THEORY

From previous sections it can be observed that the equations of motion obtained from the 2PI effective action are quite involved: nonlinear and nonlocal integro-differential equations, not readily solvable in closed form. To progress further we need to introduce approximations based on physical considerations. It is easier to proceed if one can observe and justify a separation of time scales in the relevant physical processes in question—i.e., one related to quantum processes which are usually microscopic in scale (note quantum entanglement and correlation of the system can extend to much greater scales, meso or even macro) and one related to the kinetic or transport properties, which is usually macroscopic in scale. However, this assumption of a scale separation may not be valid in mesoscopic processes (as in strongly correlated systems) or macroscopic quantum coherence effects (see footnote [1]). For those situations where a separation of macroscopic and microscopic time scales which would permit an effective kinetic theory description does *not* exist, one can adopt the *effectively open-system* framework quantified by the nPI-CTP effective action and the hierarchy of equations it generates. We begin with a discussion of the latter situation which is more demanding and general. We describe the conceptual pathway for the construction of quantum kinetic theory from the nPI effective action. Though somewhat theoretical and formally oriented, it may be of some use, as this is the first point of contact with quantum kinetic theory from the effective action approach, in the atomic and molecular physics (AMO) context (for more details on this subject see [21–24], where our discussions in the following section are based on).

Quantum kinetic theory from (nPI) effective action

It may be useful to begin by defining what we mean by a quantum kinetic theory. It contains, but supersedes, the quantum version of Boltzmann's theory. Formally it refers to the theory based on the hierarchy of coupled equations for the (relativistic) Wigner function [51] and its higher-correlation analogs, which are obtained by a Fourier transform of the relative coordinates in the Schwinger-Dyson equations [52] for the correlation functions or, alternatively, in the *master effective action* (defined as the nPI effective action when $n \to \infty$, we are dealing with $n=2$ here) whose variation yields the Schwinger-Dyson equations. This is a quantum analog of the Bogolinbov-Born-Green-Kinkwood-Yvon (BBGKY) hierarchy [53], expressed in a representation convenient for distinguishing between microscopic (quantum field-theoretic) and macroscopic (transport and relaxation) phenomena. As such, it does not require near-equilibrium conditions and, in fact, is applicable for a rather general moment expansion of the initial density matrix [21].[2]

To understand how quantum kinetic theory is derived from an nPI effective action and how it relates to the familiar Boltzmann's theory, it is perhaps helpful to examine the relation between this theory in its full generality and an effective Boltzmann description of relaxation phenomena for the one-particle distribution function of quasiparticles. In nonequilibrium statistical mechanics, as is well known [53,55], the act of truncating the classical BBGKY hierarchy does not in itself lead to irreversibility and an H theorem. One must further perform a type of *coarse graining* of the truncated, coupled equations for n-particle distribution functions. For example, if one truncates the hierarchy to include only the one-particle and two-particle distribution functions, it is the subsequent assumption that the two-particle distribution function at some initial time factorizes in terms of a product of single-particle distribution functions (which is at the heart of the molecular chaos hypothesis where the colliding particles are initially independent, but correlated after a collision), which leads to the (irreversible) Boltzmann equation. The assumption that the two-particle distribution function factorizes is an example of a type of coarse graining called *slaving* of the two-particle distribution function to the single-particle distribution function, in the language of [22]. The situation in quantum kinetic field theory is completely analogous. One may choose to work with a truncation of the hierarchy of the Wigner function and its higher-correlation analogs, or one may instead perform a slaving of, for example, the Wigner-transformed four-point function, which leads (within the context of perturbation theory) directly to the (relativistic) Boltzmann equation [21] and the usual H theorem [24]. Typically this slaving of the higher-correlation function(s) involves imposing causal boundary conditions to obtain a particular solution for the higher-correlation function(s) in terms of the lower-order correlation functions [21,22]. The truncation and subsequent slaving of the hierarchy within quantum kinetic field theory can be carried out at any desired order, as dictated by the initial conditions and relevant interactions. As with any coarse-graining procedure, in implementing the slaving of a higher-correlation–distribution function to lower-correlation–distribution functions, one is going over from a closed system to an *effectively open system,* the hallmarks of which are the emergence of dissipation [21] and noise and fluctuations [22]. This fact has led some to search for stochastic generalizations of the Boltzmann equation [56], motivated by the fact that systems in thermal equilibrium always manifest fluctuations, as embodied in the fluctuation-dissipation relation. (A derivation of the stochastic Boltzmann equation from quantum field theory can be found in [22].)

The essential point about the process of slaving of higher-correlation (or distribution) functions is that it is a step which

[2]It should be pointed out that in order to *identify* the Winger function with a distribution for quasiparticles, one must show that the density matrix has *decohered*, and this is neither guaranted nor required by the existence of a separation of macroscopic and microscopic time scales [54]

is *independent* of the assumption of macroscopic and microscopic time scales. In fact, a completely analogous procedure exists at the level of the Schwinger-Dyson equations (i.e., without Wigner transformation) for correlation functions in an interacting quantum field theory [22]. Recall that the Schwinger-Dyson equations are, in the context of nonequilibrium field theory in the Schwinger-Keldysh or closed-time-path formulation, an infinite chain of coupled dynamical equations for all order correlation functions of the quantum field. The importance of the closed-time-path formalism in nonequilibrium situations is that it ensures that the equations are causal and that the correlation functions are "in-in" expectation values in the appropriate initial quantum state or density matrix. As with the BBGKY hierarchy in nonequilibrium statistical mechanics, the common strategy is to truncate the hierarchy of correlation functions at some finite order. A general procedure has been presented for obtaining coupled equations for correlation functions at any order l in the correlation hierarchy, which involves a truncation of the master effective action at a finite order in the loop expansion [22]. By working with an l-loop-order truncation of the master effective action, one obtains a closed, time-reversal invariant set of coupled equations for the first $l+1$ correlation functions, $z=C_1$, $g=C_2, C_3, \ldots, C_{l+1}$. In general, the equation of motion for the highest-order correlation function will be linear and thus can be formally solved using Green's function methods. The existence of a unique solution depends on supplying causal boundary conditions. When the resulting solution for the highest-correlation function is then backsubstituted into the evolution equations for the other lower-order correlation functions, the resulting dynamics becomes nontime-reversal invariant and generically dissipative. As with the slaving of the higher-order Wigner-transformed correlation functions in quantum kinetic field theory, we have then gone over from a closed system (the truncated equations for correlation functions) to an effectively open system. In addition to dissipation, one expects that an effectively open system will manifest noise and fluctuations (an example of slaving the four-point function to the two-point function in the symmetry-unbroken $\lambda\Phi^4$ field theory is given in [22]). Thus a framework exists for exploring irreversibility and fluctuations within the context of a unitarily evolving quantum field theory, using the truncation and slaving of the correlation hierarchy.

While it is certainly not the only coarse-graining scheme which could be applied to an interacting quantum field, the slaving of higher correlation functions to lower-order correlation functions within a particular truncation of the correlation hierarchy, as a particular coarse-graining method, has several important benefits. First, it can be implemented in a truly nonperturbative fashion, where the variance of the mean field can be on the order of the "classical" mass (defined as the second-order derivative of the effective potential in the equation of motion for the mean field, which provides the natural time scale of the system dynamics). This necessitates a nonperturbative resummation of daisy graphs (the leading contributions in a large-$\mathcal{N}$ expansion) [14], which can be incorporated in the truncation and slaving of the correlation hierarchy in a natural way.[3] Second, the truncation of the correlation hierarchy accords with our intuition that the degrees of freedom readily accessible to physical measurements are often limited to the mean field and two-point function.

IV. SYSTEMS WHOSE DYNAMICS ADMIT TWO-TIME SEPARATION

An alternative (actually more common and easier) route to reach a kinetic theory description from n-body quantum dynamics becomes available when there is a clear separation of two time scales in the system dynamics. This is the usual textbook treatment of kinetic theory we are familiar with. The two different scales in the system are the time (or length) scale separation between the duration of a collision event (or scattering length) and the inverse collision rate (or the mean free path). For quantum processes, in the weakly interacting regime, we expect that there is also a separation between the kinetic scale of n particles (expressed in the center-of-mass coordinate) and the quantum scale (expressed in the momentum corresponding to the Fourier transform of the relative coordinates between two particle), which describes how quantum processes (such as radiative corrections) change the particle mass-energy and momenta. Using these approximations it is possible to recast the full quantum dynamics into the simpler forms of two coupled equations which constitute quantum kinetic theory, the Boltzmann equation governing the distribution functions and what is known as the gap equation for the modified dispersion relation.

For a three-dimensional uniform Bose gas the duration of a collision event τ_0 is given by the time that a particle with average velocity v spends in the interaction region measured by the range of the two-particle interaction potential. This range for a repulsive potential is typically given by the s-wave scattering length and thus $\tau_0 \approx a_s/v$. On the other hand, the inverse collision rate τ_c or time between successive collisions is approximately given by $\tau_c \approx (na_s^2 v)^{-1}$, where n is the particle density. The required separation of time scales, $\tau_c \gg \tau_0$, implies the inequality $na_s^3 \ll 1$ or, in other words, the necessary condition required for the validity of a scale separation is that the system must be in the dilute weakly interacting regime. For atoms in optical lattices the dilute weakly interacting conditions required for the scale separation is fulfilled if the average repulsive interaction energy Un, where n is the mean number of particles per lattice site, is much smaller than J, the quantum kinetic energy needed to correlate two atoms at adjacent lattice sites, or $Un/J \ll 1$.

Perhaps an intuitive way to understand the scale separation is the following. At equilibrium the correlation functions describing a homogeneous system are translationaly invariant and stationary. If the system is disturbed from equilib-

[3] At late times in the thermalization stage, when the quantum field is near equilibrium, an effective kinetic description may be justified, but will likely require resummation of hard thermal loops (see, e.g., [57]). Under such circumstances, even the evaluation of transport coefficients is nontrivial for high temperature [25,58]

rium, collisions among particles would break both invariances. However, as long as the the interaction energy per particle is smaller than the typical kinetic energy per particle, interparticle collisions are few and far between. In this case the quantum-mechanical entanglement between collision partners decays faster than the time required for the next collision to take place, particles can be considered as free between collisions, and approximate time and space translational invariance holds.

A. Coarse-graining procedure

To make the scale separation, for BEC systems at hand, it is best to perform first a gauge transformation which makes it easier to identify (and coarse-grain away) the fast variations induced by the rapid change of the condensate phase. Following Ref. [19] we introduce the gauge transformation

$$z(t_i) = e^{i\theta(t_i)}\sqrt{n_0(t_i)}, \tag{34}$$

$$g^{(\gtrless)}(t_i,t_j') = e^{i\theta(t_i)\sigma_z}\tilde{g}^{(\gtrless)}(t_i,t_j')e^{-i\theta(t_j')\sigma_z}, \tag{35}$$

where $\sqrt{n_0(t_i)}$ and $\theta(t_i)$ are real. The equations of motion are invariant under the phase transformation if we replace D_0^{-1} by $\tilde{D}_0^{-1}$:

$$\tilde{D}_0^{-1}(t_i,t_j') = [\hbar\delta_{ij}(i\sigma_z\partial_t - \partial_t\theta(t_i)) - \delta_{ij}V_i + J(e^{i\sigma_z\Delta\theta(t_{i+1/2})}\delta_{i+1j} + e^{-i\sigma_z\Delta\theta(t_{i-1/2})}\delta_{i-1j})]\delta(t-t'), \tag{36}$$

where we have introduced the definition $\Delta\theta(t_{i+1/2}) = \theta(t_{i+1}) - \theta(t_i)$. As shown in Ref. [17], in the context of the discrete Bose-Hubbard model, it is convenient to map the unitary gauge transformation to the so-called phase twist of the Hamiltonian. The twisted Hamiltonian exhibits additional phase factors $e^{\pm i\Delta\theta}$ in the hopping term, which are known as the Peierls phase factors [59,60].

The scale separation is performed by introducing the variables

$$R = (i+j)/2, \quad T = (t+t')/2, \tag{37}$$

$$r = (i-j), \quad \tau = (t-t') \tag{38}$$

For a translationally invariant system at equilibrium, the condensate density $n_0(t_i)$ is position and time independent and the propagators $g^{(\gtrless)}(t_i,t_j')$ only depend on the relative coordinates variables r and τ and are highly peaked about their zeros. If the system is disturbed by small perturbations, such as an external potential $V(t_i)$ which varies slowly in space and time, we expect for systems with scale separation that the gauge-transformed propagators $\tilde{g}^{(\gtrless)}(t_i,t_j')$ acquire a slowly varying dependence on the center-of-mass coordinates R and T but still to be peaked around the zeros of r and τ. We emphasize that the gauge-transformed, not the original, variables are the ones that are expected to be slowly varying. The reason is that even if the perturbation is slowly varying, the phase $\theta(t_i)$ can be a rapidly varying function and it can induce strong variations in the condensate amplitude and in the propagators.

Before going further, it is important to discuss the issue that by defining the spatial center-of-mass coordinates at points that strictly speaking are not lattice sites points we might be introducing unphysical degrees of freedom. We stress though that this is not the case for system with scale separation. Under the slowly varying approximation the unphysical degrees of freedom are excluded, since the functions evaluated at the R points may be thought of as the average over neighboring physical lattice sites.

We proceed now to describe the coarse-graining procedure that uses the slowly varying property of the propagators in the center-of-mass variables to simplify the equations of motion.

If the phase twist applied to the system is small, $\Delta\theta \ll \pi$, the Peierls phase factors can be written as $e^{i\Delta\theta} = 1 - i\Delta\theta - \frac{1}{2}\Delta\theta^2$. In this case, the phase factors can be physically connected to the imposition of an acceleration on the lattice and the energy change resulting from the phase twist can be attributed to the kinetic energy of the superflow generated by the acceleration. Under this picture in the context of the Bose-Hubbard model the quantity $\Delta\theta$ can be also connected, as is the gradient of the phase in non lattice systems, to the superfluid velocity:

$$\hbar v_s(t_{i+1/2}) = 2J\Delta\theta(t_{i+1/2})a_l. \tag{39}$$

with a_l the lattice spacing.

If the disturbances introduced by the perturbation are small, the superfluid velocity is expected to be a slowly varying function in space and time and to a good approximation its second-order variations can be ignored—i.e., $\Delta v_s(t) \equiv 2[v_s(t_{i+1/2}) - v_s(t_i)], \forall\ i$. Again, the quantity $v_s(t_i)$ may be thought of as the average over neighboring lattice sites: $[v_s(t_{i+1/2}) + v_s(t_{i-1/2})]/2$. Using the small-angle and slowly varying dependence of the superfluid velocity, the propagator $\tilde{D}_0^{-1}$ can thus be written in terms of the superfluid velocity as

$$\tilde{D}_0^{-1}(t_i,t_j') \approx \left[\delta_{ij}[\mathrm{i}\hbar\sigma_z\partial_t - \hbar\partial_t\theta(t_i) - V(t_i) - J\bar{v}_s^2(t_i)) + J\left(1 + \frac{\mathrm{i}}{2}\sigma_z\Delta\bar{v}_s(t)\right)[\delta_{i+1j} + \delta_{i-1j}]\right]\delta(t-t') + [Ji\sigma_z\bar{v}_s(t_i)(\delta_{i+1j} - \delta_{i-1j})]\delta(t-t'). \tag{40}$$

where we have introduced the dimensionless superfluid velocity $\bar{v}_s(t_i) \equiv \hbar v_s(t_i)/2Ja_l$.

At equilibrium, the time derivative of the phase is related to the chemical potential. Extending this identification to the nonequilibrium system we define the chemical potential as

$$\mu(t_i) = -\hbar\partial_t\theta(t_i) - J\bar{v}_s^2(t_i) - V(t_i), \tag{41}$$

If we make a change of variables $(t_i) \to (R + (r/2), T + (t/2))$ in the one-point functions $n_0(t_i)$, $\mu(t_i)$, $v_s(t_i)$, and $V(t_i)$ and use the the slowly varying dependence of the functions on the center of mass coordinates, to a good approximation the functions can be treated as continuous functions and second order variations in R and T can be neglected. Thus, they can be written as

$$n_0(t_i) = n_0(R + (r/2), T + (t/2)) = n_0(R,T) + \frac{r}{2}\partial_R n_0(R,T) + \frac{t}{2}\partial_T n_0(R,T), \quad (42)$$

$$\mu(t_i) = \mu(R + (r/2), T + (t/2)) = \mu(R,T) + \frac{r}{2}\partial_R \mu(R,T) + \frac{t}{2}\partial_T \mu(R,T), \quad (43)$$

$$v_s(t_i) = v_s(R + (r/2), T + (t/2)) = v_s(R,T) + \frac{r}{2}\partial_R v_s(R,T) + \frac{t}{2}\partial_T v_s(R,T), \quad (44)$$

$$V(t_i) = V(R + (r/2), T + (t/2)) = V(R,T) + \frac{r}{2}\partial_R V(R,T) + \frac{t}{2}\partial_T V(R,T). \quad (45)$$

Similar approximations can be made on the two-point functions by introducing a change of variables $(t_i, t_j) \rightarrow (r, \tau; R, T)$. The slowly varying dependence in R and T allow us to treat $\tilde{g}^{(\gtrless)}(r, \tau; R, T)$ as a continuous functions in the center-of-mass coordinates and neglect second-order variations in them. On the other hand, it is important to include the discrete dependence on the $r = i - j$ variables, inherent to the tight-binding Hamiltonian, in order to retain all the quantum effects introduced by the lattice which are crucial to a proper description of the system.

We now introduce a Fourier transform with respect to the relative coordinate variables. Since hereafter we use the gauge-transformed functions exclusively, the primes will be dropped to simplify the notation:

$$g^{(\gtrless)}(t_i, t_j') = g^{(\gtrless)}(r\tau; RT) \equiv -i\frac{1}{2\pi M}\sum_q \int d\omega e^{(iqa_l r - i\omega\tau)} g^{(\gtrless)}(R, q; T, \omega), \quad (46)$$

$$H(t_i, t_j') = H(r\tau; RT) \equiv -i\frac{1}{2\pi M}\sum_q \int d\omega e^{(iqa_l r - i\omega\tau)} H(R, q; T, \omega). \quad (47)$$

In the above equations M denotes the total number of lattice sites and q the lattice quasimomentum: $q = 2\pi j/(a_l M)$ with $j = 0, 1, \ldots, M-1$. Using Eq. (42) in Eq. (47) we get

$$H(R, q; T, \omega) = 2\pi M(I + \sigma_x) n_0(R,T)\delta(\omega)\delta_{q0}. \quad (48)$$

In Eq. (48), the quantity $n_0(R,T)$ is just related to the condensate density of atoms at the space time point (Ra_l, T). In Eq. (46), the upper diagonal component of the two-point function $g_{11}^{<}(R, q; T, \omega)$ corresponds to the well-known *Wigner distribution* function [51]. It can be interpreted as the density of noncondensed particles with quasimomentum q and energy $\hbar\omega$ at the position Ra_l and time T. On the other hand, $g_{11}^{>}(qR; T, \omega)$ is essentially the *density of states* available to a particle that is added to the system at (Ra_l, T) with quasimomentum q and energy $\hbar\omega$. As opposed to a normal system, the presence of the condensate gives nonzero values to the off-diagonal terms of the functions $g_{12}^{(\gtrless)}(R, q; T, \omega)$. We refer to them as the *anomalous contributions* to the respective two-point functions.

B. Generalized Boltzmann equations

The generalized Boltzmann equations can be obtained as the Fourier transform of the equations of motion for the case in which the variations in R and T are very small: in particular when the inverse propagator D_0^{-1} and the self-energies vary very little as Ra_l is changed by a characteristic excitation wavelength or T is changed by an inverse excitation energy.

If we neglect the second-order variation in T and R, as explained above, the equations of motion (27)–(30) can be approximated by

$$\left(D_0^{-1} - \Re S + \frac{i}{2}\gamma\right)H = -\frac{i}{2}[D_0^{-1}, H] + \frac{i}{2}[\Re S, H] + \frac{1}{4}[\gamma, H], \quad (49)$$

$$H\left(D_0^{-1} - \Re S - \frac{i}{2}\gamma\right) = -\frac{i}{2}[H, D_0^{-1}] + \frac{i}{2}[H, \Re S] - \frac{1}{4}[H, \gamma], \quad (50)$$

$$\left(D_0^{-1} - \Re\Sigma + \frac{i}{2}\Gamma\right)g^{(\gtrless)} - \Sigma^{(\gtrless)}\left(\Re g + \frac{i}{2}A\right) = -\frac{i}{2}[D_0^{-1}, g^{(\gtrless)}] + \frac{i}{2}[\Re\Sigma, g^{(\gtrless)}] + \frac{i}{2}[\Sigma^{(\gtrless)}, \Re g] + \frac{1}{4}[\Gamma, g^{(\gtrless)}] - \frac{1}{4}[\Sigma^{(\gtrless)}, A], \quad (51)$$

$$g^{(\gtrless)}\left(D_0^{-1} - \Re\Sigma - \frac{i}{2}\Gamma\right) - \left(\Re g - \frac{i}{2}A\right)\Sigma^{(\gtrless)} = -\frac{i}{2}[g^{(\gtrless)}, D_0^{-1}] + \frac{i}{2}[g^{(\gtrless)}, \Re\Sigma] + \frac{i}{2}[\Re g, \Sigma^{(\gtrless)}] - \frac{1}{4}[g^{(\gtrless)}, \Gamma] + \frac{1}{4}[A, \Sigma^{(\gtrless)}], \quad (52)$$

with

$$D_0^{-1}(qR; T, \omega) \equiv \{\sigma_z[\hbar\omega - \bar{v}_s(R,T)2J\sin(qa_l)] + [2J\cos(qa_l) + \mu(R,T)]I\}. \quad (53)$$

In Eqs. (49)–(52) all the quantities depend on $(qR; T\omega)$.

In the equations we have also introduced the following functions:

$$\Re S(R, q; T, \omega) = S^{HFB}(R, q; T, \omega) + \Re S^B(R, q; T, \omega), \quad (54)$$

$$\Re\Sigma(R, q; T, \omega) = \Sigma^{HFB}(R, q; T, \omega) + \Re\Sigma^B(R, q; T, \omega), \quad (55)$$

$$\Re S^B(R,q;T,\omega) = P\int \frac{d\omega'}{2\pi}\frac{\gamma(R,q;T,\omega)}{\omega-\omega'}, \tag{56}$$

$$\Re\Sigma^B(R,q;T,\omega) = P\int \frac{d\omega'}{2\pi}\frac{\Gamma(qR;T,\omega')}{\omega-\omega'}, \tag{57}$$

$$\Re g(R,q;T,\omega) = P\int \frac{d\omega'}{2\pi}\frac{A(R,q;T,\omega')}{\omega-\omega'}, \tag{58}$$

with P denoting the Cauchy principal value and $\gamma(R,q;T,\omega)$, $\Gamma(R,q;T,\omega)$, $S^{HFB}(R,q;T,\omega)$, $\Sigma^{HFB}(R,q;T,\omega)$, and $A(R,q;T,\omega)$ understood as Fourier transforms of the functions $\gamma(t_i,t_j')$, $\Gamma(t_i,t_j')$, $S^{HFB}(t_i,t_j')$, $\Sigma^{HFB}(t_i,t_j')$, and $A(t_i,t_j')$, respectively.

To approximate the discretized equations by the continuous differential equations we have also used the slowly varying dependence of the quantities on R and T. The brackets in Eqs. (49)–(52) denote the generalized Poisson brackets defined as

$$[A,B] = \frac{\partial A}{\partial\omega}\frac{\partial B}{\partial T} - \frac{\partial A}{\partial T}\frac{\partial B}{\partial\omega} + \partial_R A\partial_q B - \partial_q A\partial_R B. \tag{59}$$

Notice that even though the continuous limit has been taken at the kinetic scale, the discreteness introduced by the lattice, crucial for a correct description of the physics, is taken into account at the quantum scale, as can be seen in Eq. (53) where the free propagator has a trigonometric dependence on the quasimomentum q, characteristic of lattice-type systems. If the disturbances in the system are small enough that only long-wavelength modes are excited, $qa_l \ll 1$, the excitations only see the lower quarter of the band. In this case the free propagator reduces to

$$D_0^{-1}((q \ll 1/a_l)R;T,\omega) \approx \sigma_z[\hbar\omega - v_s(R,T)p] + \left(2J - \frac{p^2}{2m^*} + \mu(R,T)\right)I, \tag{60}$$

which is like the free propagator for a nonlattice system and the role of the lattice is just to introduce an effective mass m^*. Here $p=\hbar q$ and $m^*=\hbar^2/(2a_l^2J)$.

If we define the statistical functions [which carry a superscript (F) in paper I, Eq. (I.35)] as

$$F(R,q;T,\omega) = \frac{g^>(R,q;T,\omega) + g^<(R,q;T,\omega)}{2}, \tag{61}$$

$$\Pi(R,q;T,\omega) = \frac{\Sigma^>(R,q;T,\omega) + \Sigma^<(R,q;T,\omega)}{2}, \tag{62}$$

Eqs. (51) and (52), can be rewritten in terms of statistical and spectral functions as

$$\left(D_0^{-1} - \Re\Sigma + \frac{i}{2}\Gamma\right)F - \Pi\left(\Re g + \frac{i}{2}A\right) = -\frac{i}{2}\left\{\left[D_0^{-1} - \Re\Sigma + \frac{i}{2}\Gamma, F\right] - \left[\Pi, \Re g + \frac{i}{2}A\right]\right\}, \tag{63}$$

$$F\left(D_0^{-1} - \Re\Sigma - \frac{i}{2}\Gamma\right) - \left(\Re g - \frac{i}{2}A\right)\Pi = -\frac{i}{2}\left\{\left[F, D_0^{-1} - \Re\Sigma - \frac{i}{2}\Gamma\right] - \left[\Re g - \frac{i}{2}A, \Pi\right]\right\}, \tag{64}$$

$$(D_0^{-1} - \Re\Sigma)A - \Gamma\Re g = -\frac{i}{2}\{[D_0^{-1} - \Re\Sigma, A] - [\Gamma, \Re g]\}, \tag{65}$$

$$A(D_0^{-1} - \Re\Sigma) - \Re g\Gamma = -\frac{i}{2}\{[A, D_0^{-1} - \Re\Sigma] - [\Re g, \Gamma]\}. \tag{66}$$

Equations (49), (50), and (63)–(66) are our passage to the Boltzmann equations. They describe the state of the gas at a given time. Different from the HFB equations they include collisional integrals for binary interactions.

C. Ordinary Boltzmann equations

To progress further we can introduce more simplifications based on physical considerations. The ordinary Boltzmann equation emerges from the approximation in which the self-energies that appear on the left-hand side of Eqs. (49), (50), and (63)–(66) are handled differently from those which appear on the right. These two appearance of the self-energy play a different physical role in the description of the dynamics [18]. The self-energies on the right-hand side describe the dynamical effects of collisions—i.e., how the collisions transfer particles from one energy-momentum configuration to another. On the other hand, the self-energies on the left describe the quantum kinetic effects due to interactions—i.e., how interaction effects change the energy-momentum dispersion relations from that of free particles to a more complicated spectrum. Because these two effects are physically distinct, we can treat the left- and right-hand sides in a different way.

In the derivation of the ordinary Boltzmann equations, one completely neglects all the kinetic effects in the second-order self-energies (the dependence on T and R in the second-order self-energy terms on the right-hand side) and retain dynamical effects (T and R dependence on the left-hand side). In this way, we get the familiar Boltzmann equations which describe the particles as free particles in between collisions with a modified energy-momentum dispersion relation. It is a reasonable assumption in dilute weakly interacting gases in which the duration of a collision is very short compared to the essentially interaction-free dynamics be-

tween isolated collisions. Neglecting kinetic effects in the second-order self-energies, Eqs. (49), (50), and (63)–(66) can be approximated to

$$\left(D_0^{-1} - \Re S + \frac{i}{2}\gamma\right)H = -\frac{i}{2}[D_0^{-1} - S^{HFB}, H], \tag{67}$$

$$H\left(D_0^{-1} - \Re S - \frac{i}{2}\gamma\right) = -\frac{i}{2}[H, D_0^{-1} - S^{HFB}], \tag{68}$$

$$\left(D_0^{-1} - \Re\Sigma + \frac{i}{2}\Gamma\right)F - \Pi\left(\Re g + \frac{i}{2}A\right) = -\frac{i}{2}[D_0^{-1} - \Sigma^{HFB}, F], \tag{69}$$

$$(D_0^{-1} - \Re\Sigma)A - \Gamma\Re g = -\frac{i}{2}[D_0^{-1} - \Sigma^{HFB}, A], \tag{70}$$

$$F\left(D_0^{-1} - \Re\Sigma - \frac{i}{2}\Gamma\right) - \left(\Re g - \frac{i}{2}A\right)\Pi = -\frac{i}{2}[F, D_0^{-1} - \Sigma^{HFB}], \tag{71}$$

$$A(D_0^{-1} - \Re\Sigma) - \Re g\Gamma = -\frac{i}{2}[A, D_0^{-1} - \Sigma^{HFB}]. \tag{72}$$

If we take the trace of the sum and the difference of each one of the above equations with its Hermitian conjugate, they can be simplified to

$$\mathrm{Tr}\{(D_0^{-1} - \Re S)H\} = 0, \tag{73}$$

$$\mathrm{Tr}\{(D_0^{-1} - \Re\Sigma)F - \Pi\Re g\} = 0, \tag{74}$$

$$\mathrm{Tr}\{(D_0^{-1} - \Re\Sigma)A - \Gamma\Re g\} = 0, \tag{75}$$

$$\mathrm{Tr}[D_0^{-1} - S^{HFB}, H] = -\mathrm{Tr}(\gamma H), \tag{76}$$

$$\mathrm{Tr}[D_0^{-1} - \Sigma^{HFB}, F] = -\mathrm{Tr}(\Gamma F - \Pi A), \tag{77}$$

$$\mathrm{Tr}[D_0^{-1} - \Sigma^{HFB}, A] = 0. \tag{78}$$

Moreover, if we define the operator $\mathcal{T}rM = M_{12} + M_{21}^*$ and apply it again to the sum and the difference of each one of the equations (63)–(66) with its transpose, we also get

$$\mathrm{Re}[\mathcal{T}r\{(D_0^{-1} - \Re S)H\}] = \frac{1}{2}\,\mathrm{Im}\{\mathcal{T}r[D_0^{-1} - S^{HFB}, H] + \mathcal{T}(\gamma H)\}, \tag{79}$$

$$\mathrm{Re}[\mathcal{T}r\{(D_0^{-1} - \Re\Sigma)F - \Pi\Re g\}] = \frac{1}{2}\,\mathrm{Im}\{\mathcal{T}r[D_0^{-1} - \Sigma^{HFB}, F] + \mathcal{T}r(\Gamma F - \Pi A)\}, \tag{80}$$

$$\mathrm{Re}[\mathcal{T}r\{(D_0^{-1} - \Re\Sigma)A - \Gamma\Re g\}] = \frac{1}{2}\,\mathrm{Im}(\mathcal{T}r[D_0^{-1} - \Sigma^{HFB}, A]), \tag{81}$$

$$\mathrm{Im}[\mathcal{T}r\{(D_0^{-1} - \Re S)H\}] = -\frac{1}{2}\,\mathrm{Re}\{\mathcal{T}r[D_0^{-1} - S^{HFB}, H] + (\gamma H)\}, \tag{82}$$

$$\mathrm{Im}[\mathcal{T}r\{(D_0^{-1} - \Re\Sigma)F - \Pi\Re g\}] = -\frac{1}{2}\,\mathrm{Re}\{\mathcal{T}r[D_0^{-1} - \Sigma^{HFB}, F] + r(\Gamma F - \Pi A)\}, \tag{83}$$

$$\mathrm{Im}[\mathcal{T}r\{(D_0^{-1} - \Re\Sigma)A - \Gamma\Re g\}] = -\frac{1}{2}\,\mathrm{Re}(\mathcal{T}r[D_0^{-1} - \Sigma^{HFB}, A]), \tag{84}$$

with "Re" and "Im" denoting the real and imaginary parts. To close the set of equations, we need an equation of motion for the superfluid velocity which can be found from the definitions, Eqs. (41) and (39), to be

$$\frac{\partial \bar{v}_s(R,T)}{\partial T} = -\frac{\partial}{\partial R}\{[\mu(R,T) + V(R,T)] + J\bar{v}_s^2(R,T)\}. \tag{85}$$

Equations (73)–(84) together with Eq. (85) form a closed set of equations that describe the state of the gas at a given time. Equations (73)–(75) and (79)–(81) are usually called the *gap equations*. They describe the quantum properties of a gas which is evolving according to Boltmaznn-type equations (76)–(78) and (82)–(84). Under the derived formalism Eqs. (73)–(85) form a coupled set of equations which replace the original dynamics. The equations have to be solved self consistently for any analysis.

V. EQUILIBRIUM PROPERTIES FOR A HOMOGENEOUS SYSTEM

There are two situations in which we expect an equilibrium solution to come from the Boltzmann equations: first, when the system has never been disturbed and it remains in its equilibrium state and second, when the system has had sufficient time to relax after an applied perturbation. In this section we will show how the second-order nonequilibrium Boltzmann equations lead, in these special cases, to the linear equilibrium solutions obtained from the HFB approximation [17] upgraded with second-order corrections in U.

At equilibrium, in the absence of any external potential, the functions $g^{\gtrless}$ and H are completely independent of R and T. In this case the generalized Poisson-bracket terms are zero and Eqs. (75), (78), (81), and (78) imply that

$$A(D_0^{-1} - \Re\Sigma) - (\Re g)\Gamma = 0. \tag{86}$$

Because $\Re g(q,\omega)$ is determined by $A(q,\omega)$ as indicated in Eq. (58), Eq. (86) is satisfied when $A(q,\omega)$ is given by

$$-iA(q,\omega) = \left[D_0^{-1} - \Re\Sigma + \frac{i}{2}\Gamma\right]^{-1} - \left[D_0^{-1} - \Re\Sigma - \frac{i}{2}\Gamma\right]^{-1} \tag{87}$$

and the function $\Re g(q,\omega)$ given by

$$\Re g(q,\omega) = P\int \frac{d\omega'}{2\pi}\frac{A(q,\omega')}{\omega-\omega'} = \frac{1}{2}\left\{\left[D_0^{-1} - \Re\Sigma + \frac{i}{2}\Gamma\right]^{-1} + \left[D_0^{-1} - \Re\Sigma - \frac{i}{2}\Gamma\right]^{-1}\right\}. \tag{88}$$

From Eqs. (76), (82), (77), and (83) we also get, at equilibrium, the conditions

$$\gamma = 0, \tag{89}$$

$$\Gamma F - \Pi A = 0. \tag{90}$$

Equations (89) and (90) are just the mathematical statement of detailed balance. They represent the physical condition that at equilibrium the net rate of change of the density of particles with momentum q and energy ω is zero. Since it is always possible to write [18]

$$F(q,\omega) = \left(n_q(\omega) + \frac{1}{2}\right)A(q,\omega), \tag{91}$$

Eq. (90) can only be satisfied if

$$\Pi(q,\omega) = \left(n_q(\omega) + \frac{1}{2}\right)\Gamma(q,\omega) \tag{92}$$

is satisfied. Detailed study of the structure of the self-energy indicates that $n_q(\omega)$ is related to the Bose-Einstein thermal distribution, $n_q(\omega)=1/(e^{\beta\omega}-1)$, with β interpreted as the local inverse temperature in energy units [18,19]. In Refs. [61] the authors prove that the only translational invariant solution is the thermal.

Since H contains δ functions in momentum and energy at equilibrium, we get from Eq. (73)

$$\mu = -2J + \Re S_{11}(0,0) + \Re S_{12}(0,0). \tag{93}$$

A. Quasiparticle formalism

In the noninteracting case the diagonal terms of $A(q,\omega)$ are just δ functions with peaks at values of $\hbar\omega$ that match the possible energy difference which results from adding a single particle with quasimomentum q to the system. In the many-body system the energy spectrum is sufficiently complex so that the diagonal elements of $A(q,\omega)$ are not δ functions but instead continuous functions of ω. However, there are always sharp peaks in A. These sharp peaks represent the coherent and long-lived excitations which behave like weakly interacting particles. These excitations are called quasiparticles. From Eq. (87) it is possible to see that the quasiparticle decay rate is determined by Γ. The quasiparticle approximation is obtained by considering Γ very small for small values of ω. This assumption implies that $D^{-1}\equiv D_0^{-1}-\Re\Sigma-(i/2)\Gamma$ is essentially real with only an infinitesimal imaginary part. The zeros of D^{-1} about which A is very sharply peaked are identified with the quasiparticle energies $\hbar\omega_q$.

Using the assumption of a very small Γ and the identity

$$\lim_{\epsilon\to 0}\frac{1}{\omega-\omega'+i\epsilon} = P\frac{1}{\omega-\omega'} - i\pi\delta(\omega-\omega'), \tag{94}$$

it is possible to write the matrix components of D^{-1} as

$$D^{-1}(q,\omega) = \hbar\omega\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} - \begin{pmatrix}\mathcal{L}_{qq}(q,\omega) & \mathcal{M}_{q-q}(q,\omega)\\ \mathcal{M}^*_{q-q}(-q,-\omega) & \mathcal{L}^*_{qq}(-q,-\omega)\end{pmatrix}, \tag{95}$$

with

$$\mathcal{L}_{qq}(\omega) = -2J\cos qa_l - \mu + \Sigma_{11}^{HFB}(q,\omega) + \int\frac{d\omega'}{2\pi}\frac{\Gamma_{11}(q,\omega')}{\omega-\omega'+i\epsilon}, \tag{96}$$

$$\mathcal{M}_{q-q}(\omega) = \Sigma_{12}^{HFB}(q,\omega) + \int\frac{d\omega'}{2\pi}\frac{\Gamma_{12}(q,\omega')}{\omega-\omega'+i\epsilon}. \tag{97}$$

The quasiparticle amplitudes u_q and v_q are the solutions to the eigenvalue problem

$$\begin{pmatrix}\mathcal{L}_{qq}(q,\omega_q) & \mathcal{M}_{q-q}(q,\omega_q)\\ \mathcal{M}^*_{q-q}(-q,-\omega_q) & \mathcal{L}^*_{qq}(-q,-\omega_q)\end{pmatrix}\begin{pmatrix}u_q\\ v_q\end{pmatrix} = \hbar\omega_q\begin{pmatrix}u_q\\ -v_q\end{pmatrix} \tag{98}$$

and satisfy the normalization condition $|u_q|^2-|v_q|^2=1$. In the absence of vortices it is always possible to find an ensemble in which the amplitudes (u_q,v_q) are purely real and $u_q=u_{-q}$, $v_q=v_{-q}$. In terms of the quasiparticle amplitudes we can express the matrix components $\rho_q(\omega)$, $\varsigma_q(\omega)$, and $m_q(\omega)$ defined as the Fourier transform of ρ_{ij}, ς_{ij}, and m_{ij} respectively [see Eqs. (24) and (26)] as

$$\rho_q(\omega) = 2\pi\{u_q^2 n_q(\omega)\delta(\omega-\omega_q) + v_q^2[1+n_q(\omega)]\delta(\omega+\omega_q)\}, \tag{99}$$

$$\varsigma_q(\omega) = 2\pi\{u_q^2[1+n_q(\omega)]\delta(\omega-\omega_q) + v_q^2 n_q(\omega)\delta(\omega+\omega_q)\}, \tag{100}$$

$$m_q(\omega) = 2\pi u_q v_q\{n_q(\omega)\delta(\omega-\omega_q) + [1+n_q(\omega)]\delta(\omega+\omega_q)\}. \tag{101}$$

B. HFB approximation

Under the HFB approximation the matrices $\Re\Sigma$ and $\Re S$ are just given by Σ^{HFB} and S^{HFB} [Fourier transform of Eqs. (156) and (157)]. In terms of the quasiparticle amplitudes they can be written as

$$\Sigma^{HFB} = U\begin{pmatrix}2(n_0+\tilde{n}) & n_0+\tilde{m}\\ n_0+\tilde{m} & 2(n_0+\tilde{n})\end{pmatrix}, \tag{102}$$

$$S^{HFB} = U\begin{pmatrix}n_0+2\tilde{n} & \tilde{m}\\ \tilde{m} & n_0+2\tilde{n}\end{pmatrix}, \tag{103}$$

with

$$\tilde{n} = = \frac{1}{M}\sum_q \{[1+n_q(\omega_q)]v_q^2 + u_q^2 n_q\}, \tag{104}$$

$$\tilde{m} = \frac{1}{M}\sum_q u_q v_q [2n_q(\omega_q)+1]. \tag{105}$$

In the HFB approximation, Eqs. (98) and (93) then yield

$$\begin{pmatrix} -2J\cos(qa_l) - \mu + 2U(n_0+\tilde{n}) & U(n_0+\tilde{m}) \\ U(n_0+\tilde{m}) & -2J\cos(qa_l) - \mu + 2U(n_0+\tilde{n}) \end{pmatrix} \begin{pmatrix} u_q \\ v_q \end{pmatrix} = \hbar\omega_q \begin{pmatrix} u_q \\ -v_q \end{pmatrix}, \tag{106}$$

$$\mu = -2J + Un_0 + 2U\tilde{n} + U\tilde{m}. \tag{107}$$

As a final step, to fix the total density to n, the constraint

$$n = n_0 + \tilde{n} \tag{108}$$

has to be satisfied.

For a given density and temperature Eqs. (106)–(108) form a closed set of equations. At zero temperature, they reduce to the HFB equations derived in [17] using the quadratic approximation.

The Hugenholtz-Pines theorem states [62] that a homogeneous system at equilibrium has to fulfill

$$\mathcal{L}_{qq}(0,0) - \mathcal{M}_{q-q}(0,0) = 0. \tag{109}$$

The above equation implies that the energy spectrum of a Bose gas is gapless; i.e., there is an excitation with an energy that tends to zero in the limit of zero momentum. Mathematically the theorem implies that the two-point propagator $g(q,\omega)$ has a pole at $q=\omega=0$. Physically it reflects the fact that small rotations of the phase of the condensate wave function cost little energy (Goltstone mode of the broken symmetry). The Hugenholtz-Pines theorem is a consequence of the invariance of the mean field and the two-point propagators under a phase transformation.

The HFB approximation violates the Hugenholtz-Pines theorem

$$\mathcal{L}_{qq}(0,0) - \mathcal{M}_{q-q}(0,0) = -2U\tilde{m} \neq 0. \tag{110}$$

One way to solve the gap problem is to set the anomalous term $\tilde{m}$ to zero in HFB equations. This procedure is known as the HFB-Popov approximation. The HFB-Popov equations were first introduced by Popov [63], and at equilibrium they are consider a better approximation than the HFB equations because they yield a gapless spectrum. Nevertheless, the HFB-Popov equations are not conserving and therefore they are not appropriate to describe dynamical evolution.

C. Second-order and Beliaev approximations

When second-order terms are taken into account the matrices $\mathcal{L}_{qq}$ and $\mathcal{M}_{q-q}$ become energy dependent. For simplicity we restrict the calculations to the zero-temperature case when $n_q=0$. In terms of the quasiparticle amplitudes the contributions to the self-energy at second order are given by

$$\begin{aligned}\mathcal{M}_{q-q}(q,\omega) = {} & Un_0 + U\tilde{m} + \frac{2U^2}{\hbar M} n_0 \sum_k \left(\frac{2\mathcal{A}_k\mathcal{B}_{q-k} + 2\mathcal{C}_k\mathcal{A}_p + 2\mathcal{C}_k\mathcal{B}_{q-k} + 3\mathcal{C}_k\mathcal{C}_{q-k}}{\omega - \omega_k - \omega_{q-k} + i\epsilon} - \frac{2\mathcal{B}_k\mathcal{A}_{q-k} + 2\mathcal{C}_k\mathcal{A}_p + 2\mathcal{C}_k\mathcal{B}_{q-k} + 3\mathcal{C}_k\mathcal{C}_{q-k}}{\omega + \omega_k + \omega_{q-k} - i\epsilon} \right) \\ & + \frac{2U^2}{\hbar M^2} \sum_{k,p} \left(\frac{2\mathcal{A}_k\mathcal{B}_p\mathcal{C}_{q-k-p} + \mathcal{C}_k\mathcal{C}_p\mathcal{C}_{q-k-p}}{\omega - \omega_k - \omega_p - \omega_{q-k-p} + i\epsilon} - \frac{2\mathcal{B}_k\mathcal{A}_p\mathcal{C}_{q-k-p} + \mathcal{C}_k\mathcal{C}_p\mathcal{C}_{q-k-p}}{\omega + \omega_k + \omega_p + \omega_{q-k-p} - i\epsilon} \right),\end{aligned} \tag{111}$$

$$\begin{aligned}\mathcal{L}_{qq}(q,\omega) = {} & -2J\cos qa_l - \mu + 2Un_0 + 2U\tilde{n} + \frac{2U^2 n_0}{\hbar M} \sum_k \left(\frac{\mathcal{A}_k\mathcal{A}_{q-k} + 2\mathcal{A}_k\mathcal{B}_{q-k} + 4\mathcal{C}_k\mathcal{A}_{q-k} + 2\mathcal{C}_k\mathcal{C}_{q-k}}{\omega - \omega_k - \omega_{q-k} + i\epsilon} \right. \\ & \left. - \frac{\mathcal{B}_k\mathcal{B}_{q-k} + 2(\mathcal{B}_k\mathcal{A}_{q-k}) + 4\mathcal{C}_k\mathcal{B}_{q-k} + 2\mathcal{C}_k\mathcal{C}_{q-k}}{\omega + \omega_k + \omega_{q-k} - i\epsilon} \right) + \frac{2U^2}{\hbar M^2} \sum_{k,p} \left(\frac{\mathcal{A}_k\mathcal{A}_p\mathcal{B}_{q-k-p} + 2\mathcal{A}_k\mathcal{C}_p\mathcal{C}_{q-k-p}}{\omega - \omega_k - \omega_p - \omega_{q-k-p} + i\epsilon} \right) \\ & - \left(\frac{\mathcal{B}_k\mathcal{B}_p\mathcal{A}_{q-k-p} + 2\mathcal{B}_k\mathcal{C}_p\mathcal{C}_{q-k-p}}{\omega + \omega_k + \omega_p + \omega_{q-k-p} - i\epsilon} \right),\end{aligned} \tag{112}$$

$$\mu = -2J + Un_0 + 2U\tilde{n} + U\tilde{m} - \frac{2U^2}{\hbar M^2}\sum_{k,p}\left(\frac{2\mathcal{A}_k\mathcal{B}_p\mathcal{C}_{k+p} + 2\mathcal{B}_k\mathcal{A}_p\mathcal{C}_{k+p} + 2\mathcal{C}_k\mathcal{C}_p\mathcal{C}_{k+p}}{\omega_k + \omega_p + \omega_{k+p}}\right)$$
$$- \frac{2U^2}{\hbar M^2}\sum_{k,p}\left(\frac{2\mathcal{A}_k\mathcal{C}_p\mathcal{C}_{k+p} + \mathcal{A}_k\mathcal{A}_p\mathcal{B}_{k+p} + 2\mathcal{B}_k\mathcal{C}_p\mathcal{C}_{k+p} + \mathcal{B}_k\mathcal{B}_p\mathcal{A}_{k+p}}{\omega_k + \omega_p + \omega_{k+p}}\right), \tag{113}$$

where the quantities $\mathcal{A}$, $\mathcal{B}$, and $\mathcal{C}$ are defined as

$$\mathcal{A}_k = u_k^2, \quad \mathcal{B}_k = v_k^2, \quad \mathcal{C}_k = -u_k v_k. \tag{114}$$

The inclusion of second-order terms modifies the structure of the HFB equations. The matrix that we need to diagonalize to find the quasiparticle energies depends now on the quasiparticle mode in consideration. This means that a separate nonlinear problem must be solved for every quasiparticle state, whereas the solution of the HFB equations yields the whole quasiparticle spectrum. The matrix which is to be diagonalized also becomes intrinsically nonlocal and to solve for a quasiparticle state with quasimomentum q we have to sum over alldifferent quasimomenta. Finally, the diagonal elements are no longer equal as was always the case in all the quadratic approximations.

If we omit the second-order terms containing no condensate amplitudes, the equations that we get are the *tight-binding* version of the ones originally derived by Beliaev [46]:

$$\mathcal{M}_{q-q}(q,\omega) = Un_0 + \lambda\Delta\mathcal{M}_{q-q}(q,\omega), \tag{115}$$

$$\mathcal{L}_{qq}(q,\omega) = \epsilon[q] + Un_0 + \lambda\Delta\mathcal{L}_{qq}(q,\omega), \tag{116}$$

$$\mu = -2J + Un_0 + \lambda\Delta\mu, \tag{117}$$

with

$$\epsilon[q] = 4J\sin^2(qa_l/2), \tag{118}$$

$$\Delta\mu = 2U\tilde{n} + U\tilde{m} \tag{119}$$

and

$$\Delta\mathcal{M}_{q-q}(q,\omega) = U\tilde{m} + \frac{2U^2}{\hbar M}n_0\sum_k\left(\frac{2\mathcal{A}_k\mathcal{B}_{q-k} + 2\mathcal{C}_k\mathcal{A}_p + 2\mathcal{C}_k\mathcal{B}_{q-k} + 3\mathcal{C}_k\mathcal{C}_{q-k}}{\omega - \omega_k - \omega_{q-k} + i\epsilon} - \frac{2\mathcal{B}_k\mathcal{A}_{q-k} + 2\mathcal{C}_k\mathcal{A}_p + 2\mathcal{C}_k\mathcal{B}_{q-k} + 3\mathcal{C}_k\mathcal{C}_{q-k}}{\omega + \omega_k + \omega_{q-k} - i\epsilon}\right), \tag{120}$$

$$\Delta\mathcal{L}_{qq}(q,\omega) = -U\tilde{m} + \frac{2U^2n_0}{\hbar M}\sum_k\left(\frac{\mathcal{A}_k\mathcal{A}_{q-k} + 2\mathcal{A}_k\mathcal{B}_{q-k} + 4C_k\mathcal{A}_{q-k} + 2\mathcal{C}_k\mathcal{C}_{q-k}}{\omega - \omega_k - \omega_{q-k} + i\epsilon} - \frac{B_k\mathcal{B}_{q-k} + 2(\mathcal{B}_k\mathcal{A}_{q-k}) + 4\mathcal{C}_k\mathcal{B}_{q-k} + 2\mathcal{C}_k\mathcal{C}_{q-k}}{\omega + \omega_k + \omega_{q-k} - i\epsilon}\right), \tag{121}$$

In the above equations we introduce the parameter λ only to use it as a perturbation parameter and set to 1 at the end of the calculations.

If second-order terms are included in the theory, they change the quasiparticle spectrum not only by shifting the quasiparticle energies but also by making them complex. The imaginary part that the quasiparticle energies acquire comes from the poles of the second-order terms and it is associated with a damping rate. The physical meaning is that when the energy denominator in the second-order terms vanishes a process where a quasiparticle decays into two of lower energy is energetically allowed. This kind of damping mechanism is known as *Beliaev damping* and was calculated by Beliaev in the case of a uniform Bose superfluid [46]. In the remainder of this section we calculate the zero-temperature Beliaev damping coefficient for atoms in optical lattices using the tight-binding second-order Beliaev approximation, Eqs. (120) and (121). We follow the same ideas used by Beliaev to study the uniform system.

1. Perturbative treatment

As the starting point we assume that the net effect of second-order plus HFB terms is to introduce small corrections to the Bogoliubov–de Gennes (BdG) self-energies.[4] In this case instead of solving the equations in a self-consistent way we can replace the BdG quasiparticle energies and amplitudes in the HFB and second-order self-energy corrections to calculate the shift they introduce in the spectrum.

[4]In the translationally invariant limit the Bogoliubov–de Gennes matrix elements $\mathcal{L}_{qq}$ and $\mathcal{M}_{q-q}$ agree with the matrix elements calculted using the HFB-Popoy approximation [16,17].

The quasiparticle energies and amplitudes in the BdG approximation are given by [17]

$$\hbar\omega_q^{(0)} = \sqrt{{\varepsilon_q}^2 + 2Un_0^{(0)}\varepsilon_q}, \tag{122}$$

$$\mathcal{A}_q^{(0)} = u_q^{(0)2} = \frac{\varepsilon_q + n_0^{(0)}U + \hbar\omega_q^{(0)}}{2\hbar\omega_q^{(0)}}, \tag{123}$$

$$\mathcal{B}_q^{(0)} = v_q^{(0)2} = \frac{\varepsilon_q + n_0^{(0)}U - \hbar\omega_q^{(0)}}{2\hbar\omega_q^{(0)}}, \tag{124}$$

$$\mathcal{C}_q^{(0)} = -u_q^{(0)}v_q^{(0)} = -\frac{n_0^{(0)}U}{2\hbar\omega_q^{(0)}}, \tag{125}$$

$$\tilde{m}^{(0)} = \frac{1}{M}\sum_{q\neq 0} u_q^{(0)}v_q^{(0)}, \tag{126}$$

and

$$n = n_0^{(0)} + \frac{1}{M}\sum_{q\neq 0} v_q^{(0)2}, \tag{127}$$

with n the total density, $n=N/M$.

As shown in the last section, the HFB approximation has the problem that it has a gap in the excitation spectrum and therefore violates Pines-Hugenholtz theorem. However, as shown by Beliaev [46], when second-order Beliaev contributions are included the theory becomes gapless. This can be seen from Eqs. (120) and (121):

$$\begin{aligned}
&\Delta\mathcal{L}_{q-q}(0,0) - \Delta\mathcal{M}_{q-q}(0,0) \\
&\quad = -2U\tilde{m}^{(0)} + \frac{2U^2n_0}{\hbar M}\sum_k \left(\frac{\mathcal{A}_k^{(0)}\mathcal{A}_{-k}^{(0)} + \mathcal{B}_k^{(0)}\mathcal{B}_{-k}^{(0)} - 2\mathcal{C}_k^{(0)}\mathcal{C}_{-k}^{(0)}}{-2\omega_k^{(0)}}\right) \\
&\quad = -2U\tilde{m}^{(0)} - \frac{2U^2n_0}{\hbar M}\sum_k \frac{(u_k^{(0)2} - v_k^{(0)2})^2}{-2\omega_k^{(0)}} \\
&\quad = 2U\frac{1}{M}\sum_k \frac{Un_0}{-2\hbar\omega_k^{(0)}} - \frac{2U^2n_0}{\hbar M}\sum_k \frac{1}{-2\omega_k^{(0)}} = 0.
\end{aligned} \tag{128}$$

2. Beliaev damping

If we include HFB and second-order corrections, the quasiparticle energy shifts are given to first order in λ by

$$\begin{aligned}
\hbar\omega_q^{(1)} \equiv \delta E_q + i\gamma_q = {}& \mathcal{A}_q^{(0)}\Delta\mathcal{L}_{q-q}(q,\omega_q^{(0)}) \\
&+ \mathcal{B}_q^{(0)}\Delta\mathcal{L}_{q-q}^*(-q,-\omega_q^{(0)}) \\
&+ \mathcal{C}_q^{(0)}[\Delta\mathcal{M}_{q-q}(q,\omega_q^{(0)}) \\
&+ \Delta\mathcal{M}_{q-q}^*(-q,-\omega_q^{(0)})].
\end{aligned} \tag{129}$$

After some algebra, Eq. (129) can be written in the more convenient form

$$\begin{aligned}
\delta E_q + i\gamma_q = {}& U\tilde{m}^{(0)}(u_q^{(0)} - v_q^{(0)})^2 \\
&+ \frac{4U^2}{\hbar M}n_0^{(0)}\sum_k \left(\frac{B_{k,q-k}^2}{\omega_q^{(0)} - \omega_k^{(0)} - \omega_{q-k}^{(0)} + i\epsilon}\right. \\
&\left. - \frac{\tilde{B}_{k,q-k}^2}{\omega_q^{(0)} + \omega_k^{(0)} + \omega_{q-k}^{(0)} - i\epsilon}\right),
\end{aligned} \tag{130}$$

where the matrices $B_{k,q-k}$ and $\tilde{B}_{k,q-k}$ are defined as

$$\begin{aligned}
B_{k,q-k} = {}& u_q^{(0)}(u_k^{(0)}u_{q-k}^{(0)} - u_k^{(0)}v_{q-k}^{(0)} - v_q^{(0)}u_q^{(0)}) \\
&- v_q^{(0)}(v_k^{(0)}v_{q-k}^{(0)} - u_k^{(0)}v_{q-k}^{(0)} - v_q^{(0)}u_q^{(0)}),
\end{aligned} \tag{131}$$

$$\begin{aligned}
\tilde{B}_{k,q-k} = {}& u_q^{(0)}(v_k^{(0)}v_{q-k}^{(0)} - u_k^{(0)}v_{q-k}^{(0)} - v_q^{(0)}u_q^{(0)}) \\
&- v_q^{(0)}(u_k^{(0)}u_{q-k}^{(0)} - u_k^{(0)}v_{q-k}^{(0)} - v_q^{(0)}u_q^{(0)}).
\end{aligned} \tag{132}$$

If we replace ε_q by $\hbar q^2/2m$, the matrix elements given by Eqs. (131) and (132) reduce to the Beliaev uniform gas matrix elements (see, for example, Refs. [16,33]).

The damping coefficient can be obtained using the identity, Eq. (94), in Eq. (130). This yields

$$\gamma_q = \frac{2\pi U^2}{M\hbar}n_0^{(0)}\sum_k B_{k,q-k}^2\delta(\omega_q^{(0)} - \omega_k^{(0)} - \omega_{q-k}^{(0)}). \tag{133}$$

For a translational-invariant system at equilibrium, all quantities are T and R independent and depend only on the relative coordinates r and τ. Therefore, at equilibrium the scale separation is always valid and we can relax the condition $Un/J \ll 1$. In Ref. [17] we showed by comparison with solutions obtained by the exact diagonalization of the Bose-Hubbard Hamiltonian that for commensurate systems in the parameter regime where $(U/J) < 0.5(U/J)_c$, the BdG equations give a good description of the properties of the system. $(U/J)_c \sim dn$ is the superfluid to Mott insulator critical ratio, d the dimensionality, and n the density of the system. For systems with noncommensurate fillings, where the superfluid to Mott insulator quantum phase transition does not take place, the agreement between the BdG and exact solutions was shown to be significantly better for a larger parameter regime. Because Eq. (133) was found treating the second-order corrections as a perturbation, its validity is restricted to the parameter regime $(U/J) < 0.5(U/J)_c$, where the BdG solutions are still a good description of the system.

As opposed to the uniform system without the lattice, where for high momentum the single-particle energy (which grows as q^2) is always dominant, in the presence of the lattice, the single-particle excitation energies are always bounded by $4J$. Therefore, in the regime $Un/J > 1$,[5] the interaction term dominates for all quasimomenta and the quasiparticle amplitudes and energies can be expanded as

$$u_k^{(0)} \simeq \frac{1}{2\alpha_k} + \frac{\alpha_k}{2} + \frac{{\alpha_k}^3}{8} - \frac{{\alpha_k}^5}{8}, \tag{134}$$

[5]Notice that for large filling factors n, the parameter U_n/J can be larger than 1 but the system can be still far away from the Mott insulator critical point.

$$v_k^{(0)} \simeq \frac{1}{2\alpha_k} - \frac{\alpha_k}{2} + \frac{\alpha_k^3}{8} + \frac{\alpha_k^5}{8}, \tag{135}$$

$$\hbar\omega_k^{(0)} \simeq 2n_0^{(0)}U\left(\alpha_k^2 + \frac{1}{2}\alpha_k^6\right), \tag{136}$$

where

$$\alpha_k = \eta\left(\frac{\varepsilon_k}{J}\right)^{1/4}, \tag{137}$$

$$\eta \equiv \left(\frac{J}{2n_0^{(0)}U}\right)^{1/4}. \tag{138}$$

In the very weakly interacting regime $Un_0/J \lesssim 1$, the approximations used to derive Eqs. (134)–(136) are still valid if the quasimomentum of the excitation involved in the decay process is small, $qa_l \ll \sqrt{n_0U/J}$.

If one substitutes Eqs. (134)–(136) for the quasiparticle amplitudes in Eq. (133) and makes use of the energy conservation condition, which is approximately given by

$$\alpha_q^2 - \alpha_k^2 - \alpha_{q-k}^2 = \frac{1}{2}(\alpha_k^6 + \alpha_{q-k}^6 - \alpha_q^6), \tag{139}$$

one gets the following expression for the damping coefficient:

$$\gamma_q = \frac{9\pi}{8M}\frac{J}{n_0^{(0)}}\sum_k \sqrt{\frac{\varepsilon_q\varepsilon_k\varepsilon_{q-k}}{J^3}}\delta(\bar{e}_q - \bar{e}_k - \bar{e}_{q-k}), \tag{140}$$

with $\bar{e}_q$ the dimensionless quasiparticle energies given by $\bar{e}_q = \hbar\omega_k^{(0)}/2n_0^{(0)}U\eta^2$. When the number of lattice sites is large, to a good approximation the discrete sum can be replaced by an integral $(1/M)\Sigma_k \to a_l/2\pi\int_0^{2\pi/a_l}dk$.

For the one-dimensional system, we find that the only value of k at which the energy constraint is satisfied is when $k=q$. This value of k leads to a zero damping coefficient, and therefore in the one-dimensional system the quasiparticles become totally stable against their decay into two of lower energy. In this case higher-order decay processes have to be considered. However, the absence of Beliaev damping in one-dimensional lattices is not a particular characteristic of the lattice dispersion relation. If the damping coefficient is calculated using the one-dimensional uniform Bose gas dispersion relation, it is also found to be zero.

The extension of the expression for the Beliaev damping coefficient to higher-dimensional lattice systems can be done straightforwardly. One just has to replace the single-particle dispersion relation ε_k in Eq. (140) by the one in the specific dimension. If we assume a separable square lattice in d dimensions, with the same tunneling matrix energy J and lattice constant a_l, in all different directions we get

$$\begin{aligned}\gamma_q^{(d)} &= \frac{9\pi}{8M^d}\frac{J}{n_0^{(0)}}\sum_{\mathbf{k}} \sqrt{\frac{\varepsilon_\mathbf{q}\varepsilon_\mathbf{k}\varepsilon_{\mathbf{q}-\mathbf{k}}}{J^3}}\delta(\bar{e}_\mathbf{q} - \bar{e}_\mathbf{k} - \bar{e}_{\mathbf{q}-\mathbf{k}}) \\ &\approx \frac{9a_l^d}{16(2\pi)^{d-1}}\frac{J}{n_0^{(0)}}\int d\mathbf{k}\sqrt{\frac{\varepsilon_\mathbf{q}\varepsilon_\mathbf{k}\varepsilon_{\mathbf{q}-\mathbf{k}}}{J^3}}\delta(\bar{e}_\mathbf{q} - \bar{e}_\mathbf{k} - \bar{e}_{\mathbf{q}-\mathbf{k}}),\end{aligned} \tag{141}$$

with the definitions $\varepsilon_\mathbf{k} = 4J\Sigma_{i=1}^d \sin^2(k_i a_l/2)$, $\hbar\omega_\mathbf{k}^{(0)} \simeq 2n_0^{(0)}U(\alpha_\mathbf{k}^2 + \frac{1}{2}\alpha_\mathbf{k}^6)$, $\alpha_\mathbf{k} = \eta(\varepsilon_\mathbf{k}/J)^{1/4}$, and $\bar{e}_\mathbf{k} = \hbar\omega_\mathbf{k}^{(0)}/2n_0^{(0)}U\eta^2$.

An analytic expression for the damping coefficient can be easily obtained when the excitations involved in the decay process have a long wave number: $qa_l \ll 1$. In this parameter regime for the particular case of a three-dimensional lattice the integral yields

$$\begin{aligned}\gamma_{qa_l\ll 1}^{(d=3)} &\approx \frac{9}{32\pi}\frac{Ja_l^3}{n_0^{(0)}}\int dk d\theta \sin(\theta)k^2\sqrt{\frac{\varepsilon_\mathbf{q}\varepsilon_\mathbf{k}\varepsilon_{\mathbf{q}-\mathbf{k}}}{J^3}} \\ &\quad\times\delta(qa_l - ka_l - a_l\sqrt{p^2+q^2-2pq\cos\theta}) \\ &\approx \frac{9}{32\pi}\frac{Ja_l^5}{n_0^{(0)}}\int_0^{qa_l} dk k^2(q-p)^2 \\ &= \frac{3}{640\pi}\frac{\hbar^2 a_l^3 q^5}{m^* n_0^{(0)}},\end{aligned} \tag{142}$$

with $m^* = \hbar^2/(2Ja_l^2)$ the effective mass. In the long-wavelength limit, or phonon regime, the damping coefficient in the lattice reduces to the well-known result first obtained by Beliaev in the phonon regime, with the mass replaced by an effective mass.

Outside the phonon regime, the analytic evaluation of the integral is more complicated because of the energy conservation constraint. In the uniform gas case, which has a simpler quasiparticle spectrum, it has been shown that there is a finite threshold momentum q^* such that the decay of an excitation is impossible if $q > q^*$ [64]. We expect that the trigonometric dependence on the quasimomentum of the quasiparticle dispersion relation in lattice-type systems makes the energy conservation constraint even harder to fulfill. In Ref. [65] the authors calculated the finite-temperature Landau damping coefficient in a one-dimensional optical lattice and showed the disappearance of Landau damping when $Un_0/J \geqslant 6$.

VI. CONCLUSIONS

In this work we extended our previous studies of the dynamics of bosonic atoms confined in optical potentials. Here, starting from the 2PI-CTP equations of motion, derived in paper I from the Bose-Hubbard Hamiltonian, we show how the complicated nonlocal, non-Markovian integro-differential equations can be simplified and reduced to the standard equations of kinetic theory. Specifically, by using a two-time separation condition, valid in dilute weakly interacting systems not very far away from equilibrium, we recast the full quantum dynamics into two coupled sets of equations: the first being set of Boltzmann equations governing the distribution functions and the second being a set of gap

equations describing the modified dispersion relation. We conclude here with three remarks on some general features of this problem and our approach.

First, a remark on quantum kinetic theory in discrete versus continuous systems: Even though we work with a system described by the Bose-Hubbard Hamiltonian, the assumption that the propagators are slowly varying in the center-of-mass coordinates permits one to map the discrete tight-binding equations into a set of continuous differential equations in the center-of-mass coordinates. For this reason the dynamical equations of motion we derived for discrete systems look very similar to previous kinetic equations derived for continuous systems. On the other hand, to include all the relevant dynamical effects introduced by the lattice potential, we kept the discrete character of the tight-binding Hamiltonian in the equations for the relative coordinates, as manifested in the gap equations which exhibit a dispersion relation different from the homogeneous Bose gas system.

Second, the last section of this work was dedicated to a study of quantum equilibrium solutions. By using the quasiparticle approximation, we recovered from the kinetic equations the linear HFB corrections to the self-energy plus second-order corrections. We showed how one can one obtain a tight-binding version of the well-known Beliaev equations by neglecting the condensate-independent second-order terms in the self-energy. We used these equations to derive expressions for the zero-temperature Beliaev damping coefficient in lattice systems in certain parameter regimes. In particular, we showed that for long-wavelength excitations, the damping coefficient in a three-dimensional lattice reduces to the one calculated for a uniform Bose gas in the phonon regime, but with the mass replaced by the effective mass induced by the lattice.

A final remark on the purpose of this work. It is not meant to be a mere academic exercise in our demonstration of how Boltzmann-like equations are obtained from the effective action and how equilibrium solutions can be obtained from the full quantal solutions. In making explicit the simplifying assumptions en route starting from first principles, we identify limitations and the applicability of a kinetic theory formulation for describing the quantum dynamics of many-body lattice systems. This serves to identify the range of validity and the parameter regimes where the underlying assumptions leading to these simplified kinetic equations can become unreliable. We view this effort as having both theoretical and practical significance in seeking a proper description of such systems and better understanding of their behavior—theoretical in scrutinizing the practicing kinetic theories in existence and practical in providing the correct parameters for comparison with experiments.

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APPENDIX: HFB AND FULL SECOND-ORDER SELF-ENERGIES

To explicitly evaluate S^{HFB}, Σ^{HFB}, S, and Σ we need the expressions for $\Gamma_2^{(1)}[g]$ and $\Gamma_2^{(2)}[\mathbf{z},g]$. In Ref. [12] [Eqs. (I43) and (I53)] we showed they are given by

$$\Gamma_2^{(1)}[g] = \frac{U}{8}\sum_i \int_C dt\{\mathrm{Tr}[g(t_i,t_i)]\mathrm{Tr}[g(t_i,t_i)] + 2\,\mathrm{Tr}[g(t_i,t_i)\mathcal{G}(t_i,t_i)]\}, \tag{A1}$$

$$\begin{aligned}\Gamma_2^{(2)}[H,g] = &-\left(\frac{U}{2}\right)^2\sum_{i,j}\int_C dtdt'\{\mathrm{Tr}[H(t_i,t_j')\mathcal{G}(t_i,t_j')] \\ &\times\mathrm{Tr}[g(t_i,t_j')\mathcal{G}(t_i,t_j')] + 2\,\mathrm{Tr}[H(t_i,t_j') \\ &\times\mathcal{G}(t_i,t_j')g(t_i,t_j')\mathcal{G}(t_i,t_j')]\} \\ &-\left(\frac{U}{4}\right)^2\sum_{i,j}\int_C dtdt'\{\mathrm{Tr}[g(t_i,t_j')\mathcal{G}(t_i,t_j')] \\ &\times\mathrm{Tr}[g(t_i,t_j')\mathcal{G}(t_i,t_j')] + 2\,\mathrm{Tr}[g(t_i,t_j') \\ &\times\mathcal{G}(t_i,t_j')g(t_i,t_j')\mathcal{G}(t_i,t_j')]\},\end{aligned} \tag{A2}$$

with

$$\mathcal{G}(t_i,t_j') \equiv \sigma_x(g(t_i,t_j'))^{\mathsf{T}}\sigma_x, \tag{A3}$$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tag{A4}$$

where the symbol g^{T} means the transpose of g.

Using Eqs. (A1) and (A2) in the definitions, Eqs. (13)–(16), the self-energies S^{HFB}, Σ^{HFB}, S, and Σ can be written as

$$\Sigma^{HFB}(t_i,t_j') \equiv i\frac{U}{2}\{\mathrm{Tr}[H(t_i,t_j') + g(t_i,t_j')]I + 2[H(t_i,t_j') + g(t_i,t_j')]\}\delta(t-t')\delta_{ij,}, \tag{A5}$$

$$S^{HFB}(t_i,t_j') \equiv i\frac{U}{2}\{\mathrm{Tr}[H(t_i,t_j') + g(t_i,t_j')]I + 2g(t_i,t_j')\}\delta(t-t')\delta_{ij}, \tag{A6}$$

$$S(t_i,t_j') \equiv -\frac{U^2}{2}\{g(t_i,t_j')\mathrm{Tr}[g(t_i,t_j')\mathcal{G}(t_i,t_j')] + 2g(t_i,t_j')\mathcal{G}(t_i,t_j')g(t_i,t_j')\}, \tag{A7}$$

$$\begin{aligned}\Sigma(t_i,t_j') \equiv &-\frac{U^2}{2}\{H(t_i,t_j')\mathrm{Tr}[g(t_i,t_j')\mathcal{G}(t_i,t_j')] \\ &+ 2H(t_i,t_j')\mathcal{G}(t_i,t_j')g(t_i,t_j') + 2g(t_i,t_j')[H(t_j',t_i)g(t_i,t_j') \\ &+ \mathcal{G}(t_i,t_j')H(t_i,t_j')\end{aligned}$$

$$+\mathcal{G}(t_i,t_j')g(t_i,t_j')]g(t_i,t_j')\mathrm{Tr}[H(t_j',t_i)g(t_i,t_j') + \mathcal{G}(t_i,t_j')H(t_i,t_j') + \mathcal{G}(t_i,t_j')g(t_i,t_j')]\}. \tag{A8}$$

Utilizing the CTP decompositions in Eqs. (A7) and (A8) one gets

$$S^{(\gtrless)}(t_i,t_j') \equiv -\frac{U^2}{2}\{g^{(\gtrless)}(t_i,t_j')\mathrm{Tr}[g^{(\gtrless)}(t_i,t_j')g^{(\gtrless)}(t_j',t_i)] + 2g^{(\gtrless)}(t_i,t_j')g^{(\gtrless)}(t_j',t_i)g^{(\gtrless)}(t_i,t_j')\}, \tag{A9}$$

$$\Sigma^{(\gtrless)}(t_i,t_j') \equiv -\frac{U^2}{2}\{H(t_i,t_j')\mathrm{Tr}[g^{(\gtrless)}(t_i,t_j')g^{(\gtrless)}(t_j',t_i)] + 2H(t_i,t_j')g^{(\gtrless)}(t_j',t_i)g^{(\gtrless)}(t_i,t_j') + 2g^{(\gtrless)}(t_i,t_j') \times[H(t_j',t_i)g^{(\gtrless)}(t_i,t_j') + g^{(\gtrless)}(t_j',t_i)H(t_i,t_j') + g^{(\gtrless)} \times(t_j',t_i)g^{(\gtrless)}(t_i,t_j')]g^{(\gtrless)}(t_i,t_j')\mathrm{Tr}[H(t_j',t_i)g^{(\gtrless)}(t_i,t_j') + g^{(\gtrless)}(t_j',t_i)H(t_i,t_j') + g^{(\gtrless)}(t_j',t_i)g^{(\gtrless)}(t_i,t_j')]\}. \tag{A10}$$

It is convenient to decompose the above equations in their matrix components. Using the definitions, Eqs. (24)–(26), into the self-energies yields

$$S_{11}^{>}(t_i,t_j') = -2\mathrm{i}U^2\varsigma_{ij}(2m_{ij}m_{ji}^{*} + \varsigma_{ij}\rho_{ji}), \tag{A11}$$

$$S_{12}^{>}(t_i,t_j') = -2\mathrm{i}U^2m_{ij}(m_{ij}m_{ji}^{*} + 2\varsigma_{ij}\rho_{ji}), \tag{A12}$$

$$S_{11}^{<}(t_i,t_j') = -2\mathrm{i}U^2\rho_{ij}(2m_{ji}m_{ij}^{*} + \varsigma_{ji}\rho_{ij}), \tag{A13}$$

$$S_{12}^{<}(t_i,t_j') = -2\mathrm{i}U^2m_{ji}(m_{ij}m_{ji}^{*} + 2\varsigma_{ji}\rho_{ij}), \tag{A14}$$

$$\Sigma^{HFB}(t_i,t_j') = U\begin{pmatrix} 2|z_i|^2 + \rho_{ii} + \varsigma_{ii} & z_i^2 + m_{ii} \\ z_i^{*2} + m_{ii}^{*} & 2|z_i|^2 + \rho_{ii} + \varsigma_{ii}\end{pmatrix}\delta(t-t')\delta_{ij}, \tag{A15}$$

$$S^{HFB}(t_i,t_j') = U\begin{pmatrix} |z_i|^2 + \rho_{ii} + \varsigma_{ii} & m_{ii} \\ m_{ii}^{*} & |z_i|^2 + \rho_{ii} + \varsigma_{ii}\end{pmatrix}\delta(t-t')\delta_{ij}, \tag{A16}$$

$$\Sigma_{11}^{>}(t_i,t_j') = -2\mathrm{i}U^2(\rho_{ji}\varsigma_{ij}{}^2 + 2m_{ij}\varsigma_{ij}m_{ji}{}^{*} + 2\varsigma_{ij}m_{ji}{}^{*}z_iz_j + \varsigma_{ij}{}^2z_jz_i{}^{*} + 2\rho_{ji}\varsigma_{ij}z_iz_j{}^{*} + 2m_{ij}m_{ji}{}^{*}z_j{}^{*}z_i + 2m_{ij}\varsigma_{ij}z_i{}^{*}z_j{}^{*}), \tag{A17}$$

$$\Sigma_{12}^{>}(t_i,t_j') = -2\mathrm{i}U^2(2\rho_{ji}m_{ij}\varsigma_{ij} + 2\rho_{ji}\varsigma_{ij}z_iz_j + m_{ij}{}^2m_{ji}{}^{*} + 2m_{ij}z_iz_jm_{ji}{}^{*} + 2m_{ij}\varsigma_{ij}z_jz_i{}^{*} + 2\rho_{ji}m_{ij}z_iz_j{}^{*} + m_{ij}{}^2z_i{}^{*}z_j{}^{*}), \tag{A18}$$

$$\Sigma_{11}^{<}(t_i,t_j') = -2\mathrm{i}U^2(\rho_{ij}{}^2\varsigma_{ji} + 2\rho_{ij}m_{ji}m_{ij}{}^{*} + 2\rho_{ij}z_iz_jm_{ij}{}^{*} + \rho_{ij}^2z_jz_i{}^{*} + 2\rho_{ij}\varsigma_{ji}z_iz_j{}^{*} + 2m_{ji}z_im_{ij}{}^{*}z_j{}^{*} + 2\rho_{ij}m_{ji}z_i{}^{*}z_j{}^{*}), \tag{A19}$$

$$\Sigma_{12}^{<}(t_i,t_j') = -2\mathrm{i}U^2(2\rho_{ij}m_{ji}\varsigma_{ji} + 2\rho_{ij}\varsigma_{ji}z_iz_j + m_{ji}{}^2m_{ij}{}^{*} + 2m_{ji}z_iz_jm_{ij}{}^{*} + 2\rho_{ij}m_{ji}z_jz_i{}^{*} + 2m_{ji}\varsigma_{ji}z_iz_j{}^{*} + m_{ji}{}^2z_i{}^{*}z_j{}^{*}), \tag{A20}$$

and

$$S_{22}^{\gtrless}(t_i,t_j') = S_{11}^{\gtrless}(t_i,t_j')\{\rho_{ij} \rightleftarrows \varsigma_{ij}\}, \tag{A21}$$

$$S_{21}^{\gtrless}(t_i,t_j') = S_{12}^{\gtrless}(t_i,t_j')\{m_{ji} \rightleftarrows m_{ij}{}^{*}\}, \tag{A22}$$

$$\Sigma_{22}^{\gtrless}(t_i,t_j') = \Sigma_{11}^{\gtrless}(t_i,t_j')\{z_i \rightleftarrows z_j, \rho_{ij} \rightleftarrows \tilde{\rho}_{ij}\}, \tag{A23}$$

$$\Sigma_{21}^{\gtrless}(t_i,t_j') = \Sigma_{12}^{\gtrless}(t_i,t_j')\{z_i \rightleftarrows z_j{}^{*}, m_{ji} \rightleftarrows m_{ij}{}^{*}\}. \tag{A24}$$

In the equations we have omitted the explicit time dependence of the functions ρ, ς, and m to shorten the equations. In all the equations the index j have to be understood as always linked to t' while the index i as always linked to t [for example, m_{ji} should be understood as $m_{ji}(t',t)$].

The above expressions for the self-energy, which contain two-particle-irreducible diagrams up to second order in the interaction strength, agree exactly with those used in Refs. [28,30,32].

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