Quantum many-body interactions in the presence of disordered potentials

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Abstract: The time evolution of the quantum nonequilibrium states of many-body particles is described with a set of hierarchies of quantum kinetic equations with quantum wave functions. A collision term is obtained in terms of two-body interactions in the mean-field with a disordered potential, which is proposed for the first time. The implications and the limits of applicability of the resulting kinetic equations are discussed.

Key words: Quantum kinetics, density matrices, disordered potentials, mean field

1. Introduction

The study of quantum many-body systems is still quite far from being complete. One of the outstanding problems in this domain is to understand the effect of disordered potentials. In collision theory, disordered potentials are associated with random scattering of particles, such as the scattering of photons in atmospheric dust and the scattering of electrons in disordered crystals. This is very important for our understanding of the behavior of quantum systems such as quantum phase transitions in disordered potentials [1,2], Anderson localization of noninteracting particles [3], coherent back scattering [4], and so on. For the description of a disordered system, an arbitrary physical observable is averaged with respect to the distribution function of the system under consideration. For this purpose, quantum mechanical phase space wave functions are widely used for the formulation and solution of scattering problems. The use of the quantum mechanical phase space wave function is simply based on the quantum generalization of the classical Boltzmann N-particle distribution function [5]. As is well known, the 6N-dimensional phase space of the position and momentum coordinates cannot be used in quantum mechanics because of the restrictions imposed by the uncertainty principle that forbids states with simultaneously definite coordinates q_i and momentum p_i. The first quasiprobability distribution function similar to the classical phase space distribution function was proposed by Wigner [6] to study quantum corrections to classical mechanics, which can be obtained by Fourier transform on relative coordinates $\vec{r}$, with center-of-mass coordinates $\vec{R}$:

$$f(\vec{p}, \vec{R}, t) = \int \frac{d^3\,\vec{r}}{(2\pi)^3}\, e^{i\vec{p}.\vec{r}} \Psi^*(\vec{R} - \tfrac{1}{2}\,\vec{r},\ \vec{R} + \tfrac{1}{2}\,\vec{r}\,;t)\Psi(\vec{R} + \tfrac{1}{2}\,\vec{r},\ \vec{R} - \tfrac{1}{2}\,\vec{r}\,;t), \tag{1}$$

where $f(\vec{p}, \vec{R}, t)$ is the Wigner distribution function, from which one may write the probability density in coordinate space as follows:

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$$\int d^3\vec{p}\, f(\vec{p},\vec{R},t) = \int \frac{d^3\,\vec{r}}{(2\pi)^3}(2\pi)^3\delta(\vec{r}\,)\psi^*(\vec{R}-\frac{1}{2}\vec{r})\,\psi(\vec{R}+\frac{1}{2}\vec{r}) = \left|\Psi(\vec{r},t)\right|^2, \tag{2}$$

and, using the Fourier transform, one may obtain the probability density in momentum space as follows:

$$\int d^3\vec{R}\, f(\vec{p},\vec{R},t) = \left|C(\vec{p},t)\right|^2, \;\; with\; \psi(\vec{R},t) = \int \frac{d^3\,\vec{p}}{(2\pi)^{3/2}}C(\vec{p},t)\,e^{i\vec{p}.\vec{r}}. \tag{3}$$

In this case, one may verify that $f* = f$, but f can be negative in some regions of phase space. All the resulting wave functions and their phase-space Schrödinger equations governing the time evolution of these wave functions are equivalent to the quantum mechanical Liouville–von Neumann equation for the Wigner distribution function interpreted as a certain Fourier transform of the quantum mechanical density matrix. Phase space formulation has been widely used in the nonequilibrium theory of quantum states [7,8] and in nonlinear optics [9,10]. One may also consider various distribution functions existing in the literature, such as those of Glauber [11,12], Sudarshan [13], and Husumi [14]. The choice of the most suitable distribution function is a matter of convenience with the system under consideration. However, this short manuscript is intended to facilitate a discussion of disordered quantum states in terms of density matrices (in quantum wave functions), rather than propose a quantum correction. While some of the results in this paper have been derived previously (see, for example, [5,15]), there exist some derivations when the disordered potentials are on the agenda, presented for the first time.

2. Quantum nonequilibrium states in the absence of disordered potentials

For orientation, let us start with a transparent derivation of quantum kinetic equations in this section, with the aim of facilitating a discussion in terms of disordered potentials in the next section. The state of an N-particle system can be defined by a symmetric (bosonic) or antisymmetric (fermionic) N-particle density matrix $\rho^{(N)}$, which is taken to be normalized to N!. The density matrices are described by the wave function of the state of an N-particle system, which can be expanded in a series of orthonormal basis functions:

$$\psi(x) = \sum_n C_n \Psi_n(x)\,,\; with\;\; \psi^{(i)}(x) = \sum_n C_n^{(i)}\psi_n(x) \; for\; each\; possible\; state. \tag{4}$$

The average value of an arbitrary operator O in any state is given by:

$$O^{(i)} = \sum_n \sum_m C_n^{(i)*}\, C_m^{(i)}\, O_{n\,m}. \tag{5}$$

Let the system have the probability Pi of being in the state $\psi(i)(x)$, and then we have:

$$< O > = \sum_i P_i O^{(i)} = \sum_i P_i \sum_n \sum_m C_n^{(i)*}C_m^{(i)}O_{nm} = \sum_n \sum_m O_{n\,m}\,\rho_{n\,m}\,,\;\; with\;\; \sum_i P_i = 1. \tag{6}$$

Now we can introduce a matrix defined by:

$$\rho_{mn} = \sum_i P_i C_m^{(i)}C_n^{i*} = \int d\vec{x}\,\psi_m^*(x)\,\rho\,\psi_n(x),\;\; < O > \; = \sum_n < n\,|O\rho\,|\,n> = Tr(O\rho), \tag{7}$$

$$Tr(\rho) = \sum_i \sum_n P_i C_n^{(i)*}C_n^{(i)} = \sum_i P_i = 1. \tag{8}$$

Taking the time derivative of $\rho(t)$ in the interaction picture one may obtain the Liouville–von Neumann equation, which describes the time evolution of a nonequilibrium quantum state consisting of N-particles, as follows:

$$i\hbar\frac{\partial\rho(t)}{\partial t} = [H, \rho(t)], \tag{9}$$

where the N-particle density matrix $\rho(t) = \exp(\frac{-iHt}{\hbar})\rho(\frac{iHt}{\hbar})$ is obtained by using a unitary transformation generated by the Hamiltonian operator $H = \sum\limits_{i=1}^{N} K_i + \sum\limits_{i<j=1}^{N} V_{ij}$. The average value of any arbitrary observable $\tilde{O}$ can be expressed as a sum of the diagonal elements (or trace) of the matrix $\tilde{O}\rho(t)$ as $<\tilde{O}> = Tr(\tilde{O}\rho)$. Introducing the reduced one-particle, two-particle,..., n-particle density matrices in analogy to the hierarchy of classical phase space distribution functions [16], we obtain the following hierarchy of density matrices:

$$
\begin{aligned}
\rho^{(1)}(1) &= \frac{N!}{(N-1)!}Tr_{(2,3,\dots,N)}\rho^{(N)}(1,2,...,N) \\
\rho^{(2)}(1,2) &= \frac{N!}{(N-2)!}Tr_{(3,4,\dots,N)}\rho^{(N)}(1,2,...,N) \\
&\quad\dots\dots\quad\quad\dots\dots\dots\dots \\
\rho^{(n)}(1,2,...,n) &= \frac{N!}{(N-n)!}Tr_{(n+1,\dots,N)}\rho^{(N)}(1,2,...,N).
\end{aligned}
\tag{10}
$$

Taking the traces of both sides of this equation over the particles (1, 2, ..., n), and using Eq. (8), e.g., $\text{Tr}_{(1,2,...,N)}\rho^{(N)} = 1$, one gets the following relation:

$$Tr_{(1,2,...,n)}\rho^{(n)}(1,2,...,n) = \frac{N!}{(N-n)!}. \tag{11}$$

Taking the appropriate traces in Eq. (9), and using Eq. (11), and then multiplying both sides with $N!/(N--1)!$, we obtain the following set of kinetic equations, which describe the time evolution of one-particle, two-particle, ..., and n-particle reduced density matrices:

$$i\hbar\frac{\partial}{\partial t}\rho^{(n)}(1,2,...,n) = \sum\limits_{i=1}^{n}\left[K_i, \rho^{(n)}(1,2,...,n)\right] + \sum\limits_{i<j=1}^{n}\left[V_{ij}, \rho^{(n)}(1,2,...,n)\right]$$

$$+ Tr_{(n+1)}\sum\limits_{i=1}^{n}\left[V_{i(n+1)}, \rho^{(n+1)}(1,2,...,n+1)\right]. \tag{12}$$

This set of coupled equations is called the BBGKY-hierarchy of density matrices, and it expresses $\rho(n)$ in terms of $\rho(n+1)$. One should find a suitable approximation to uncouple this hierarchy in order to obtain a closed equation for $\rho(n)$. The kinetic equations can be obtained by appropriate truncation in Eq. (12). Taking $n = 1$, one gets the kinetic equation correspondingly:

$$i\hbar\frac{\partial}{\partial t}\rho^{(1)}(1) = \left[K_1, \rho^{(1)}(1)\right] + Tr_{(2)}\left[V_{12}, \rho^{(2)}(1,2)\right]. \tag{13}$$

These equations describe the time evolution of a single-particle density matrix with two-body interaction term. The physical interpretation of Eq. (13) is that the time derivative of the single-particle density matrix can

be written as the sum of a flux term and a collision term expressed in terms of two-body interactions and a two-particle density matrix. For the solution of Eq. (13), this equation should be uncoupled, and this can be done by means of the Boltzmann molecular chaos assumption (for sufficiently dilute systems, the N-particle density matrix can be written as a product of one-particle density matrices), writing the two-particle density matrix in terms of one-particle density matrices as follows:

$$\rho_0^{(2)}(1,2) = \rho^{(1)}(1)\rho^{(1)}(2). \tag{14}$$

Introducing this assumption in Eq. (13), we get the time-dependent Hartree–Fock equation for the one-particle density matrix:

$$i\hbar\frac{\partial}{\partial t}\rho^{(1)}(1) = \left[K_1 + U_1, \rho^{(1)}(1) \right]. \tag{15}$$

Here U_1 is the mean-field, which has the following form:

$$U_1 = Tr_{(2)}V_{12}\rho^{(1)}(2). \tag{16}$$

Eq. (15) may be generalized by incorporating the residual two-body interactions. Truncation of Eq. (12) at $n = 2$ provides us with the following kinetic equation that includes the three-body collisions:

$$i\hbar\frac{\partial}{\partial t}\rho^{(2)}(1,2) = \left[K_1 + K_2 + V_{12}, \rho^{(2)}(1,2) \right] + Tr_{(3)}\left[V_{13} + V_{23}, \rho^{(3)}(1,2,3) \right]. \tag{17}$$

If the three-body collisions are neglected in the dilute gas limit, then Eq. (17) takes the uncoupled form:

$$i\hbar\frac{\partial}{\partial t}\rho^{(2)}(1,2) = \left[K_1 + K_2 + V_{12}, \rho^{(2)}(1,2) \right]. \tag{18}$$

In this case, this equation is valid only in the case of collisions with particle 1 and particle 2. Following a similar method used by Snider [2], we obtain an appropriate solution to Eq. (18) according to the formal scattering theory of Lippmann and Schwinger [17] as follows:

$$\rho_0^{(2)}(1,2) = \Omega_{12}^{(+)}\rho^{(1)}(1)\rho^{(1)}(2)\Omega_{12}^{(+)*} , \tag{19}$$

where $\Omega_{12}^{(+)}$ denotes the Moller operator [18] defined by:

$$\Omega_{12}^{(+)} = \lim_{\tau\to-\infty} \exp\left[i(K_1 + K_2 + V_{12})\frac{\tau}{\hbar} \right] \exp\left[-i(K_1 + K_2)\frac{\tau}{\hbar} \right]. \tag{20}$$

Inserting Eq. (19) into Eq. (13), one obtains the quantum mechanical kinetic equation in terms of one-particle density matrices as follows:

$$i\hbar\frac{\partial}{\partial t}\rho^{(1)}(1) = \left[K_1, \rho^{(1)}(1) \right] + Tr_{(2)}\left[V_{12}, \Omega_{12}^{(+)}\rho^{(1)}(1)\rho^{(1)}(2)\Omega_{12}^{(+)*} \right]. \tag{21}$$

Thus, we have obtained a collision term due to the two-body collisions in the absence of disordered potentials, in terms of one-particle density matrices. This equation is valid for the ensemble-averaged single particle density in the limit when the correlation time of two-body collisions is much smaller than the mean-free time between collisions (dilute gas limit). As a result, taking the limit $\tau \to -\infty$ in Eq. (20), we can obtain a Markovian equation by neglecting the memory effects in the collision term. It involves the quantum mechanical operators V_{12} and $\Omega^{(+)}$, from which one may express the collisional results, such as the free-nucleon T-matrix T_{12}. Then the Moller operator can be written in terms of T_{12}, which obeys the Lippmann–Schwinger equation.

3. Many-body interactions in a disordered potential

As was pointed out in the introduction, disordered potentials complicate the physical system under consideration and they provide a new scattering scenario for the many-particle states. The dynamics of the system, in this case, are governed by the kinetic energy, disordered potential, and interaction energy. Disregarding the strength of the disorder (weak or strong) for the moment, let us discuss the new forms of the quantum kinetic equations in case of the presence of the disordered potentials. In this respect, we propose a one-particle disordered potential denoted by $V(\vec{r}_i)$, and then the Hamiltonian of an N-particle system can be written as follows:

$$H = \sum_{i=1}^{N} K_i + \sum_{i=1}^{N} V(\vec{r}_i) + \sum_{i<j=1}^{N} V_{ij} \tag{22}$$

where K_i denotes the kinetic energy of each particle and V_{ij} denotes the two-body interaction potential. Inserting this Hamiltonian term in the Liouville–von Neumann equation (Eq. (9)), we get the quantum kinetic equation for the N-particle density matrix, which cannot be solved due to the great number of degrees of freedom. However, one may obtain approximate solutions in terms of single-particle density matrices in the dilute gas limit. In this case, a key insight was suggested by Boltzmann: an N-particle density matrix may be written in terms of the product of single-particle density matrices, the so-called molecular chaos assumption (Boltzmann's Stosszahlansatz). Now let us consider the Liouville–von Neumann equation (Eq. (9)), which describes the time evolution of the one-particle density matrix. Taking n = 1, in the existence of the disordered potential, and following the previous approaches used for the derivation of Eq. (15), we obtain

$$i\hbar\frac{\partial}{\partial t}\rho^{(1)}(1) = \left[K_1 + V(\vec{r}_1) + U_1, \ \rho^{(1)}(1) \right], \tag{23}$$

where $V(r_1)$ is the disordered potential (for one particle), and U_1 is the mean field due to the two-body interactions as defined by Eq. (16). Taking n = 2 in Eq. (12) with Eqs. (11) and (9), we obtain

$$i\hbar\frac{\partial}{\partial t}\rho^{(2)}(1,2) = \left[K_1 + K_2 + V(\vec{r}_1) + V(\vec{r}_2) + V_{12}, \ \rho^{(2)}(1,2) \right]$$
$$+ Tr_{(3)} \left[V_{13} + V_{23}, \rho^{(3)}(1,2,3) \right]. \tag{24}$$

In the dilute gas limit, the possibility of the triple collisions is very small and for this reason three-body terms in Eq. (25) can be neglected. Thus, Eq. (25) takes the following form:

$$i\hbar\frac{\partial}{\partial t}\rho^{(2)}(1,2) = \left[K_1 + K_2 + V(\vec{r}_1) + V(\vec{r}_2) + V_{12}, \ \rho^{(2)}(1,2) \right]. \tag{25}$$

This uncoupled equation describes the time evolution of the two-particle density matrix in the disordered potential. This equation is valid only during the collision between particles 1 and 2. In order to obtain a collision term for single-particle density matrix $\rho^{(1)}(1)$, one should achieve an approximation that provides a possibility of expressing pair density matrix $\rho^{(2)}(1,2)$ in terms of single-particle density matrices, such as the molecular chaos assumption given by Eq. (14). In this context, several approximations have been developed in the existing literature to obtain a solution for the kinetic equations in terms of single-particle density matrices. For example, in [19], it was shown that phase space techniques based on Wigner representation provide an

approximate description of dilute ultracold Bose gases at zero temperature, where quantum fluctuations are important, and at finite temperature, where thermal fluctuations dominate. In these approaches, quantum field evolution can be represented by using equations of motion of a form similar to that of the Gross–Pitaevskii equation. For implementing this formalism, they present numerical techniques for a wide range of phenomena, using the fact that the Wigner function exists for any density matrix for quantum states [20]. For example, in [21], a simple approximation of the quantum kinetic equation is derived on the basis of the assumption that the density operator of the total system can be factorized into a condensate density operator for the Bose condensate band and an operator for the noncondensed modes, which is assumed to be in thermal equilibrium. It was also shown that the limiting cases of this equation include the Gross–Pitaevskii equation.

4. Conclusions

A transparent derivation of a set of hierarchies of quantum kinetic equations, which describe the time evolution of the quantum nonequilibrium states of a many-particle system in the presence of disordered potentials, has been introduced. These N-particle equations provide us with a full description in terms of the complete density matrix and single-density matrices. A collision term, from which one may express the collisional results, is obtained in terms of single-particle density matrices. We show that one may obtain a set of quantum kinetic equations of motion by taking higher-order truncations in this hierarchy for one-body, two-body, . . ., n-body interactions, and we show how one may express a two-particle density matrix in terms of single-particle density matrices by means of the molecular chaos assumption in the dilute gas limit, where the three-body collisions may be neglected. However, as the density tends to increase, the three-body, four-body, . . ., n-body interactions become important, and this would bring complications to the solutions of these equations due to the great number of degrees of freedom. Quantum kinetic equations with density matrices have been extensively used to describe the equilibrium and nonequilibrium dynamics of Bose–Einstein condensates in dilute ultracold gases, at the mean-field level, by means of the Gross–Pitaevskii equation, which is a limiting case of the presently derived kinetic equations of single-particle density matrices in disordered potentials (see, for example, [21–26]; effects of the disordered potentials were discussed extensively in these references).

Another approach for the solution of quantum kinetic equations is the path integral method of nonequilibrium quantum statistics of coherent states, which seems to be very useful for applications on quantum optics, chemical reactions, heavy-ion collisions, lasers, and other collective excitations (see, for a review, [15]). In the path integral method, the Hamiltonian is written in terms of creation and annihilation operators for Bose and Fermi systems, and integration for the kernel of the density matrices is performed in the functional space of periodic functions for the Bose systems and antiperiodic functions for the Fermi systems. The generating functionals for the Green functions are written in the form of the path integrals, which are generally not Gaussian, and these integrals are calculated by perturbation theory. The perturbation methods with truncated potentials were also found to be successful to produce the properties of many body systems [15,27]. Hopefully, this formulation in terms of the density matrices may be a useful tool for further analysis of the effects of the disordered potentials, which would be worthwhile to provide a better understanding of the localization.

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