

Generalized T–Matrix Approximation in Quantum Kinetic Equations

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Received 9 February 2001, in final form 23 May 2001

Abstract

The correct description of relaxation processes in *strongly correlated* plasmas requires quantum kinetic equations which go beyond the usual Boltzmann equation. Here, the Kadanoff–Baym equations (KBE) in the frame of real-time Green’s functions have a high degree of generality. We present a possibility to solve the KBE in T–matrix approximation by solving the Lippmann–Schwinger equation using a separable potential ansatz. Results for the T–matrix are shown for a hydrogen plasma for several screening parameters.

1 Introduction

The theoretical description of the nonequilibrium behavior of strongly correlated plasmas is connected with some essential complications. Conventional kinetic equations, i.e. equations of the Boltzmann type, which have been traditionally used in nonequilibrium many-particle physics show several disadvantages. For example, they lead to ideal conservation laws, e.g., conservation of the kinetic or quasiparticle energy only instead of the sum of kinetic and potential energy. Of course, this cannot describe the physics of strongly coupled systems correctly. Moreover, as they do not contain contributions of initial binary correlations, these equations are valid only for times larger than the correlation time of the system.

Among the generalizations, the Kadanoff–Baym equations (KBE) in the framework of nonequilibrium Green’s functions are of special interest. Due to their two-time structure they allow to calculate statistical and spectral properties at the same time and, thus, avoid the well-known consistency problems of single-time kinetic equations which always need the spectral function as an input.

Up to now numerical investigations using the KBE [1] were restricted to simple approximations for the self-energy, e.g. the second order Born approximation, e.g. [2]. However, strong correlations in the system require self-energies which go beyond the Born level, i.e., in T–matrix approximation. While for the equilibrium case there exist a number of attempts to calculate the T–matrix, its inclusion into the nonequilibrium calculations, and especially into the KBE, is still a challenging task.

In the following section, we shortly repeat the generalized KBE containing a contribution of initial correlations [3, 4, 5]. Afterwards we present a possibility to solve the Lippmann–Schwinger equation for the T–matrix using a separable potential ansatz.

2 Kadanoff–Baym equations. Self-energy

The Kadanoff–Baym equations describe the time-evolution of the two-time correlation functions $g^{\lessgtr}$ which are defined as

$$g^>(1, 1') = \frac{1}{i\hbar} \langle \psi(1) \psi^\dagger(1') \rangle, \quad g^<(1, 1') = \pm \frac{1}{i\hbar} \langle \psi^\dagger(1') \psi(1) \rangle, \quad (1)$$

with $1 = \mathbf{r}_1, s_1^3, t_1$. In momentum representation the KBE read

$$\begin{aligned} \left(i\hbar \frac{\partial}{\partial t} - \frac{p_1^2}{2m} - \Sigma^{\text{HF}}(\mathbf{p}_1, t) \right) g^{\lessgtr}(\mathbf{p}_1, t, t') \\ = \int_{t_0}^t d\bar{t} \{ \Sigma^>(\mathbf{p}_1, t, \bar{t}) - \Sigma^<(\mathbf{p}_1, t, \bar{t}) \} g^{\lessgtr}(\mathbf{p}_1, \bar{t}, t') \\ - \int_{t_0}^{t'} d\bar{t} \Sigma^{\lessgtr}(\mathbf{p}_1, t, \bar{t}) \{ g^>(\mathbf{p}_1, \bar{t}, t') - g^<(\mathbf{p}_1, \bar{t}, t') \} \end{aligned} \quad (2)$$

together with its adjoint equation. The self-energy is of the following structure [4, 5]:

$$\Sigma^{\lessgtr} = \Sigma_C^{\lessgtr} + \Sigma^{\text{IN}} \quad (3)$$

with the correlation term $\Sigma_C^{\lessgtr}$ and the time-local initial correlation term Σ^{IN} . Notice that $\Sigma_C^{\lessgtr}$ contains contributions of initial correlations, too [4, 5].

Due to the two-time character of the correlation functions $g^{\lessgtr}$ they do not only contain the statistical (one-particle) properties, e.g. Wigner function

$$f(\mathbf{p}, t) = (\pm i\hbar) g^<(\mathbf{p}, t, t')|_{t'=t}, \quad (4)$$

particle density, and kinetic energy, but also two-particle properties such as the potential energy, and, moreover, the spectral information in form of the spectral function,

$$A(\mathbf{p}, t, t') = i\hbar [g^>(\mathbf{p}, t, t') - g^<(\mathbf{p}, t, t')]. \quad (5)$$

What remains is to choose a suitable approximation for the self-energy which will be done in the following section.

3 Generalized T–matrix approximation

A generalization of the T–matrix approximation to arbitrary binary correlations being present in the system initially has been derived in ref. [5]. We only want to repeat the result for the self-energy contribution free of initial correlations. It reads in momentum representation

$$\begin{aligned} \Sigma^{\lessgtr}(\mathbf{p}_1, t, t') = \pm 2 \frac{(i\hbar)^2}{\mathcal{V}} \int d\bar{t} d\bar{t}' \int \frac{d\mathbf{p}_2}{(2\pi\hbar)^3} \frac{d\bar{\mathbf{p}}_1}{(2\pi\hbar)^3} \frac{d\bar{\mathbf{p}}_2}{(2\pi\hbar)^3} \\ \times \langle \mathbf{p}_1 \mathbf{p}_2 | T^{\text{R}}(t, \bar{t}) | \bar{\mathbf{p}}_2 \bar{\mathbf{p}}_1 \rangle g^{\lessgtr}(\bar{\mathbf{p}}_1, \bar{t}, \bar{t}') g^{\lessgtr}(\bar{\mathbf{p}}_2, \bar{t}, \bar{t}') \langle \bar{\mathbf{p}}_1 \bar{\mathbf{p}}_2 | T^{\text{A}}(\bar{t}', t) | \mathbf{p}_2 \mathbf{p}_1 \rangle g^{\lessgtr}(\mathbf{p}_2, t', t). \end{aligned} \quad (6)$$

All contributions to the self-energy can be expressed by the retarded and advanced T-matrices $T^{\text{R/A}}$. They obey a Lippmann–Schwinger equation (LSE) the structure of which is in complete analogy to the LSE known from quantum scattering theory,

$$\begin{aligned} \langle \mathbf{p}_1 \mathbf{p}_2 | T_{ab}^{\text{R/A}}(t, t') | \mathbf{p}'_2 \mathbf{p}'_1 \rangle &= \langle \mathbf{p}_1 \mathbf{p}_2 | V_{ab} | \mathbf{p}'_2 \mathbf{p}'_1 \rangle \delta(t - t') + i\hbar \int \frac{d\bar{\mathbf{p}}_1}{(2\pi\hbar)^3} \frac{d\bar{\mathbf{p}}_2}{(2\pi\hbar)^3} \int d\bar{t} \\ &\times \langle \mathbf{p}_1 \mathbf{p}_2 | V_{ab} | \bar{\mathbf{p}}_2 \bar{\mathbf{p}}_1 \rangle \tilde{\mathcal{G}}_{ab}^{\text{R/A}}(\bar{\mathbf{p}}_1, \bar{\mathbf{p}}_2; t, \bar{t}) \langle \bar{\mathbf{p}}_1 \bar{\mathbf{p}}_2 | T_{ab}^{\text{R/A}}(\bar{t}, t') | \mathbf{p}'_2 \mathbf{p}'_1 \rangle, \end{aligned} \quad (7)$$

with the propagators

$$\begin{aligned} \tilde{\mathcal{G}}_{ab}^{\text{R/A}}(\mathbf{p}_1, \mathbf{p}_2; t, t') &= \pm \Theta[\pm(t - t')] \\ &\times \{g_a^>(\mathbf{p}_1, t, t')g_b^>(\mathbf{p}_2, t, t') - g_a^<(\mathbf{p}_1, t, t')g_b^<(\mathbf{p}_2, t, t')\}, \end{aligned} \quad (8)$$

and the matrix element of the potential

$$\langle \mathbf{p}_1 \mathbf{p}_2 | V_{ab} | \mathbf{p}'_2 \mathbf{p}'_1 \rangle = Z_a Z_b V(\mathbf{p}_1 - \mathbf{p}'_1)(2\pi\hbar)^3 \delta(\mathbf{p}_1 + \mathbf{p}_2 - \mathbf{p}'_1 - \mathbf{p}'_2). \quad (9)$$

Thus, the determination of the self-energy requires the solution of eq. (7) self-consistently with the KBE (2). However, due to the complicated momentum structure of eq. (7) (dependence of the T-matrix on four momenta!), up to now, a numerical solution has not been possible. The goal of any treatment of the LSE, therefore, is to find simplifications of the momentum structure.

3.1 Separable potential ansatz

In order to follow the last idea, we introduce the ansatz for the potential to be separable in the momenta,

$$V(\mathbf{p}_1 - \mathbf{p}'_1) = \sum_{i,j} \alpha_{ij} \phi_i(\mathbf{p}_1) \phi_j(\mathbf{p}'_1), \quad (10)$$

where, in the following, we restrict ourselves to the special case of a potential of rank 1 ($i = j = 1$):

$$V(\mathbf{p}_1 - \mathbf{p}'_1) = \alpha \phi(\mathbf{p}_1) \phi(\mathbf{p}'_1). \quad (11)$$

With this ansatz, the LSE (7) is transformed into a simpler integral equation

$$\Omega_{ab}^{\text{R/A}}(\mathbf{p}_1 + \mathbf{p}_2; t, t') = \delta(t - t') + \int d\bar{t} I_{ab}^{\text{R/A}}(\mathbf{p}_1 + \mathbf{p}_2; t, \bar{t}) \Omega_{ab}^{\text{R/A}}(\mathbf{p}_1 + \mathbf{p}_2; \bar{t}, t') \quad (12)$$

with

$$I_{ab}^{\text{R/A}}(\mathbf{p}_1 + \mathbf{p}_2; t, t') = i\hbar \alpha Z_a Z_b \int \frac{d\bar{\mathbf{p}}_1}{(2\pi\hbar)^3} [\phi(\bar{\mathbf{p}}_1)]^2 \tilde{\mathcal{G}}_{ab}^{\text{R/A}}(\bar{\mathbf{p}}_1, \mathbf{p}_1 + \mathbf{p}_2 - \bar{\mathbf{p}}_1; t, t'). \quad (13)$$

Then the T-matrix can be presented as

$$\langle \mathbf{p}_1 \mathbf{p}_2 | T_{ab}^{\text{R/A}}(t, t') | \mathbf{p}'_2 \mathbf{p}'_1 \rangle = \langle \mathbf{p}_1 \mathbf{p}_2 | V_{ab} | \mathbf{p}'_2 \mathbf{p}'_1 \rangle \Omega_{ab}^{\text{R/A}}(\mathbf{p}_1 + \mathbf{p}_2; t, t'). \quad (14)$$

This representation shows that the function $\Omega^{\text{R/A}}$ can be regarded as an analogue to the well-known Møller operator of quantum scattering theory. Equations (2,6,12-14) form a closed system which is still too complicated to be solved self-consistently. Therefore, we apply additional approximations: [i] the generalized Kadanoff–Baym ansatz [6] for $\tilde{\mathcal{G}}_{ab}^{\text{R/A}}$ with free particle propagators, [ii] neglect of Pauli blocking, and [iii] a separable potential which reproduces the hydrogen 1s bound state [$\alpha = \frac{1}{2}$ and $\phi(\mathbf{p}) = \sqrt{V(\mathbf{p})}$, cf. eq. (11)], where $V(\mathbf{p})$ is the statically screened Coulomb (Debye) potential. With these simplifications, eq. (13) can be solved analytically yielding for $\Omega^{\text{R/A}}$ in frequency space, after separating the momentum dependence

$$\Omega_{ab}^{\text{R/A}}(\omega) = \tilde{\Omega}_{ab}^{\text{R/A}} \left(\omega - \frac{(\mathbf{p}_1 + \mathbf{p}_2)^2}{2M\hbar} \right), \quad (15)$$

$$\tilde{\Omega}_{ab}^{\text{R/A}}(\omega) = \frac{1}{1 - \frac{\mu e^2}{\hbar} \frac{1}{\hbar\kappa - \sqrt{-2\mu\hbar(\omega \pm i\epsilon)}}}, \quad (16)$$

with $M = m_a + m_b$ and $\mu^{-1} = m_a^{-1} + m_b^{-1}$. With eqs. (14-16) the T-matrix is determined for arbitrary momenta. In the following, we will apply the obtained equations to a hydrogen plasma.

4 Numerical approach and outlook

As an application, we consider a hydrogen plasma where the mass ratio is $m_p/m_e = 1836.15$. This allows us to treat the protons as classical particles assuming further that [i] protons have Maxwellian distributions, [ii] for them Pauli blocking is negligible, and [iii] the generalized Kadanoff–Baym ansatz with free-particle propagators for the correlation functions $g_p^{\geq}$ can be applied. Furthermore, we neglect initial correlations.¹ With these simplifications, the $e-p$ scattering contribution to the electron self-energy is given by

$$\Sigma_{ep,T}^{\geq}(\mathbf{p}_e, t, t') = \int d\bar{t} d\bar{t}' \tilde{\Omega}_{ep}^{\text{R}}(t - \bar{t}) \Sigma_{ep,\text{Born}}^{\geq}(\mathbf{p}_e, \bar{t}, \bar{t}') \tilde{\Omega}_{ep}^{\text{A}}(\bar{t}' - t'), \quad (17)$$

$$\begin{aligned} \text{with } \Sigma_{ep,\text{Born}}^{\geq}(\mathbf{p}_e, t, t') &= n_p \int \frac{d\mathbf{q}}{(2\pi\hbar)^3} |V(\mathbf{q})|^2 g_e^{\geq}(\mathbf{p}_e + \mathbf{q}, t, t') \\ &\times e^{-\frac{i}{\hbar} \frac{q^2}{2m_p}(t-t')} e^{-\frac{kTq^2}{2m_p\hbar^2}(t-t')^2}. \end{aligned} \quad (18)$$

Thus, in this approximation, the T-matrix self-energy is given by the Born approximation result multiplied by two Møller functions $\tilde{\Omega}^{\text{R}}$ and $\tilde{\Omega}^{\text{A}}$. These functions contain the full scattering information, including the possibility of the formation of bound $e-p$ pairs. This is shown in Fig. 1 where $\tilde{\Omega}^{\text{R}} - 1$ is plotted for various values of the screening parameter κ . The bound states appear in the imaginary part (b) as peaks at the effective binding energy. In addition, the maximum at positive energies represents the continuum of scattering states. One clearly sees that with increasing screening (κ), the binding energy is reduced, and the peak eventually merges with the continuum for $\kappa \equiv 1/r_D = 1/a_B$, which is just the Mott effect.

¹For the inclusion of initial correlations in second Born approximation see refs. [3, 4].

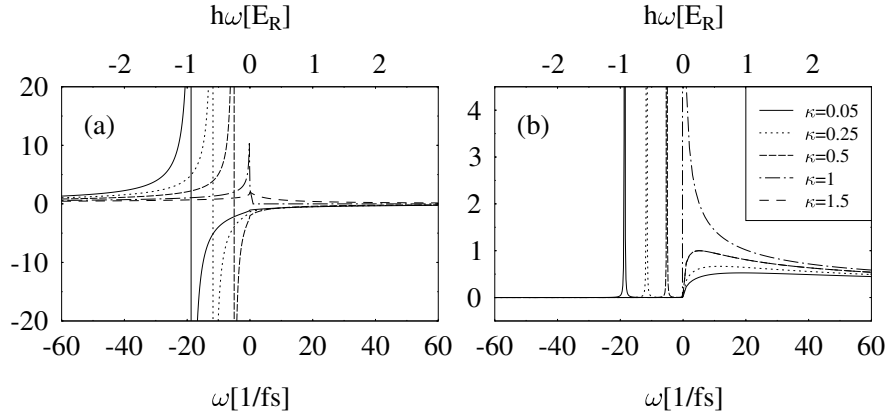


Fig. 1: Real part (a) and imaginary part (b) of $\tilde{\Omega}^R - 1$, eq. (16) for hydrogen for several inverse screening lengths κ (in units of a_B^{-1}). With increasing κ , i.e., increasing density (or decreasing temperature), the bound state peak moves and finally merges with the continuum.

In summary, we have developed a new approach which allows to solve the Kadanoff–Baym equations with self-energies in T–matrix approximation. The Lippmann–Schwinger equation for the retarded and advanced T–matrices has been solved by using a separable potential ansatz leading to self-energies, eq. (17) which are numerically tractable. We have shown that this approximation reproduces the bound and scattering spectrum of hydrogen, where the quantitative agreement can be improved by increasing the rank of the separable potential, eq. (10). Time-dependent solutions of the KBE with the self-energies (17) are in progress and will be reported in a forthcoming publication.

Acknowledgements

This work was supported by the Deutsche Forschungsgemeinschaft (SFB 198) and a grant for CPU time at the HLRZ Jülich.

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