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Generalized Kadanoff–Baym Theory for Non–Equilibrium Many–Body Systems in External Fields. An Effective Multi–Band Approach

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Abstract

The Kadanoff–Baym approach (two–time nonequilibrium Green's functions approach) is extended to charged particle systems in external fields. It is shown that its combination with an effective multi–band picture[1] yields a powerful theoretical and numerical method to describe correlated many–body systems in nonequilibrium.

1 Kadanoff–Baym approach to relaxation in many–body systems

Ultrafast relaxation processes in quantum many–body systems are presently attracting much interest, especially due to the development of femtosecond lasers and their rapidly growing availabilty and application. The theoretical description of relaxation on a femtosecond scale is difficult because it requires to take into account complex processes, such as the buildup of correlations and of dynamical screening or the formation of bound states. This is far beyond the scope of conventional (Boltzmann–type) kinetic equations; among the possible generalizations, the two–time Kadanoff–Baym approach [2] was found to be advantageous [3] due to its remarkable internal consistency because all approximations are determined by a single function (the selfenergy Σ).

After investigating the general properties of the KBE, e.g. [3], we now extend this approach to correlated many–particle systems under the influence of quite general external fields U.

2 External fields. Generalized Interband KBE

We consider an N–particle system with the Hamilton operator

$$\hat{H}(t) = \hat{H}_{sys} + \sum_i \hat{U}(\hat{x}_i, \hat{p}_i, t), \quad i = 1, \ldots N, \tag{1}$$

where the system Hamiltonian is $\hat{H}_{sys} = \sum_i \hat{H}_i(\hat{p}_i) + \sum_{i<j} V_{ij}$, with $\hat{H}_i$ and V_{ij} being the one–particle Hamiltonian and the binary interaction potential, respectively. The external potential $\hat{U}$ may be for instance (but is not limited to) a transverse electromagnetic field or a longitudinal electric field. The best known and analyzed example, e.g. [4, 5], are semiconductors subject to a low intensity laser field which may excite electrons from one energy band (μ_1) to another (μ_2). Here, the appropriate theoretical basis is given by the *interband KBE* which are the coupled equations of motion for the one–particle two–time correlation matrix $G_{\mu_1\mu_2}(t_1 t_2)$ describing the *intra*band ($\mu_1 = \mu_2$) and *inter*band ($\mu_1 \neq \mu_2$) propagation of electrons. For the explicit equations and numerical solutions, see [3, 6].

[1] This concept was first presented at the German Physical Society (DPG) Spring meeting, Regensburg, March 1998 [1].

On the other hand, it is well known that an interband transition of a *single electron* can equivalently be described as the *two-particle process* of creation of an electron-hole pair in the conduction/valence band. The corresponding theoretical description is given by the Bethe-Salpeter equation for the *two-particle* (four-point) Green's function $G_{[eh]}$ [7]. It fully describes the *propagation of an e-h pair*, including the correlations between the particles and - if taken in ladder approximation - also the possibility to form a bound state (incoherent exciton). From the view of this complicated theory, it must be a surprise that excitonic phenomena are described also in the simpler *interband KBE* discussed above where, moreover, the selfenergies Σ have to be taken only in Hartree-Fock approximation, e.g. [4, 5]. In the following, we will consider the correspondence of the two approaches more in detail and discuss possible generalizations of the *one-particle multi-band* description to other many-body systems.

Let us consider the KBE (Dyson equation) for the nonequilibrium Green's functions for system (1) which we write in integral form on the Keldysh contour,

$$G = G_0^{[0]} + G_0^{[0]} (\Sigma + U) G, \tag{2}$$

where the full Green's function G is generated from the uncorrelated (subscript "0") and field-free (superscript "[0]" denotes $U \equiv 0$) Green's function $G_0^{[0]}$ under the action of Σ and U. To separate the correlation and field effects, we rewrite (2) according to

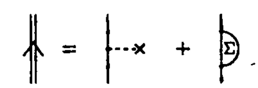
$$G^{[0]} = G_0^{[0]} + G_0^{[0]} \Sigma^{[0]} G^{[0]}, \tag{3}$$

$$G = G^{[0]} + G^{[0]} \left(\Sigma^{[1]} + \Sigma^{[2]} + \ldots + U \right) G, \tag{4}$$

where $G^{[0]}$ is the *correlated field-free* Green's function. The field appears now only in the second equation, where we also took into account that U gives rise to additional contributions to Σ, which are written as an expansion in powers of the field with $\Sigma^{[m]} \sim U^m$. While these equations may be analyzed for arbitrary field strength, e.g. [4], the comparison with the Bethe-Salpeter theory is performed most easily for weak fields.

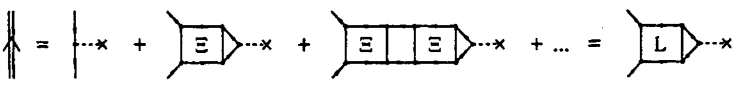
3 Weak field. Linear response

If U is small so that, for all $m > 1$, $\Sigma^{[m]} \ll \Sigma^{[1]}$, Eq. (4) may be linearized in the field leading to $G^{[1]} = G^{[0]} \left(\Sigma^{[1]} + U\right) G^{[0]}$, which may be written diagrammatically as



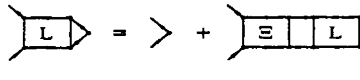
(5)

where a single full line stands for $iG^{[0]}$, a double line for $iG^{[1]}$ and a dashed line for $(-i)U$. Expressing the first order selfenergy by a field-free four-point vertex $\Xi^{[0]}$ times a first order Green's function, $\Sigma^{[1]} = \Xi^{[0]} G^{[1]}$, [8], Eq. (5) can be solved by iteration,



(6)

where we defined a generalized retarded susceptibility L^R. Its equation of motion follows immediately from Eq. (6), and is just the Bethe-Salpeter equation:



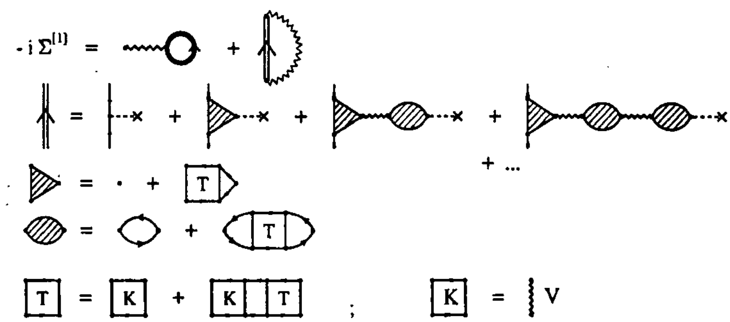
(7)

Thus, we have established a direct relation between the *one-particle* and *two-particle* approaches given by equations (5) and (7), respectively. Moreover, we have derived a one to one correspondence between the central quantities of the two theories, the single–particle selfenergy $\Sigma^{[0]}$ and the two–particle vertex $\Xi^{[0]}$. In choosing an approximation for $\Sigma^{[0]}$, we immediately may derive the equivalent result for $\Xi^{[0]}$. This will be demonstrated below for two important examples.

4 Examples for $\Sigma^{[0]}$ and corresponding results for $\Sigma^{[1]}$ and $\Xi^{[0]}$

The procedure of deriving $\Gamma^{[0]}$ for a given $\Sigma^{[0]}$ is straightforward. First, one has to determine $\Sigma^{[1]}$ which follows from $\Sigma^{[0]}$ by replacing one $G^{[0]}$ by a full $G^{[1]}$ (each $G^{[0]}$ gives rise to a separate class of diagrams), see e.g. Eq. (8). Next, with this $\Sigma^{[1]}$, Eq. (5) is solved by iteration, starting with $G^{[1]} = G^{[0]}UG^{[0]}$ and so on. Finally, the appearing diagrams have to be summed and classified.

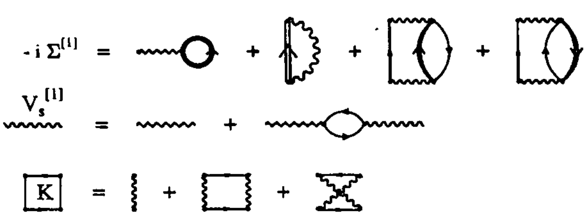
I. We start from the Hartree–Fock approximation for $\Sigma^{[0]}$. The result is



(8)

where V is the Coulomb potential and T the T-matrix. Thus, already the Hartree–Fock selfenergy in the interband KBE gives rise to a Bethe Salpeter equation on the T-matrix + ring diagrams level, and, therefore, includes bound states, as mentioned above.

II. Now the interesting question arises, which consequences for $\Gamma^{[0]}$ has the inclusion of correlations in $\Sigma^{[0]}$. Using the random phase approximation we obtain a result of the same form, except for a more general function K,



(9)

which involves the dynamic potential $V_s^{[0]}$ and vertex corrections. This leads to a dynamically screened T-matrix T, cf. Eq. (8).

5 Conclusions

In this paper, we have established the correspondence between the one and two–particle descriptions of nonequilibrium many–body systems and demonstrated that the one–particle multi–band approach is able to describe the same phenomena with a much simpler approximation. Two restrictions apply: the KBE approach crucially depends on the existence of the field U and allows only to reproduce the retarded two–particle quantities (i.e. the response properties) and, furthermore, the exact correspondence exists only for the linear response case. However, the crucial point is beyond this formal correspondence and lies in its far reaching practical consequences: It opens the possibility to switch from one description to the other whenever needed, taking advantage of favorable properties of both. In particular, one can use the KB approach with its known consistency properties to include into the Bethe–Salpeter theory correlations in a systematic way, thereby fully preserving conservation laws, sum rules etc. Furthermore, the Kadanoff–Baym approach, being now feasible for direct numerical solution [3, 6], may be used to compute the time dependent excitation and relaxation dynamics of many–body systems subject to a field, fully taking into account correlation effects on a very high level, such as the dynamically screened ladder approximation.

While, for weak fields, the solution $G^{[1]}$ is essentially the band-off-diagonal Green's function, the calculations may be directly extended to strong fields where also the band occupations will be affected by the field.

Interestingly, this approach may be extended to other many-body systems, if there exists a field U the action of which consists in creating a particle (particle-hole, particle-antiparticle) pair. For example, it allows for an efficient analysis of nonlinear plasma oscillations in nonideal quantum systems [9].

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[8] In linear response, the familiar definition $\Xi \sim \delta\Sigma/\delta G$ is equivalent to $\Sigma^{[1]}/G^{[1]}$.

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