Real-time Kadanoff-Baym approach to nuclear response functions

H S Köhler$^1$ and N H Kwong$^2$

$^1$ Physics Department, University of Arizona, Tucson, Arizona 85721, USA
$^2$ College of Optical Sciences, University of Arizona, Tucson, Arizona, 85721, USA

E-mail: kohler@physics.arizona.edu, kwong@optics.arizona.edu

Abstract. Linear density response functions are calculated for symmetric nuclear matter of normal density by time-evolving two-time Green’s functions in real time. Of particular interest is the effect of correlations. The system is therefore initially time-evolved with a collision term calculated in a direct Born approximation until fully correlated. An external time-dependent potential is then applied. The ensuing density fluctuations are recorded to calculate the density response. This method was previously used by Kwong and Bonitz for studying plasma oscillations in a correlated electron gas. The energy-weighted sum-rule for the response function is guaranteed by using conserving self-energy insertions as the method then generates the full vertex-functions. These can alternatively be calculated by solving a Bethe-Salpeter equation as done in works by Bozek et al. The (first order) mean field is derived from a momentum-dependent (non-local) interaction while 2$^{nd}$ order self-energies are calculated using a particle-hole two-body effective (or residual) interaction given by a gaussian local potential.

We show results of calculations of the response function $S(\omega,q_0)$ for $q_0 = 0.2, 0.4$ and $0.8$ fm$^{-1}$. Comparison is made with the nucleons being un-correlated i.e. with only the first order mean field included.

We discuss the relation of our work with the Landau quasi-particle theory as applied to nuclear systems by Babu and Brown and followers.

1. Introduction

Response functions, the response of a many-body system to an external perturbation is instrumental in our understanding of the properties and interactions involved in the excitations of the system. In the study of nuclear systems these response functions are of particular interest when it comes to calculate the mean free path and absorpton of neutrinos in a neutron gas [1, 2], a subject of interest in astrophysical studies. [3, 4] It has been shown that the neutrino interaction in a nuclear medium is very sensitive to the afore-mentioned response function, with the mean free path $\lambda$ given by:

$$\frac{1}{\lambda(k_\nu,T)} = \frac{G_F^2}{16\pi^2} \int dk_3 [c_V^2(1 + \cos\theta)S^{(0)}(q,T) + c_A^2(3 - \cos\theta)S^{(1)}(q,T)]$$ (1)

with $k_\nu$ and $k_3$ being initial and final neutrino momenta, $\theta$ the scattering angle. $S^{(0,1)}$ are the spin 0 and 1 response functions. $G_F$ is the Fermi constant and $c_V,A$ the coupling constants.

This report concerns the calculation of linear density response functions for symmetric nuclear matter. Of particular interest here is the effect of correlations i.e. dressed propagators and...
collision-terms. It was shown by Baym and Kadanoff [5] that, if one wishes to construct the linear response function with dressed equilibrium Green’s functions, appropriate vertex corrections to the polarization bubble are necessary to guarantee the preservation of the local continuity equation for the particle density and current in the excited system, which in turn implies the satisfaction of the energy-weighted sum rule. This problem has traditionally involved solving a Bethe-Salpeter equation to calculate these vertex corrections. Such a calculation was done by Bozek for nuclear matter[6] and further applied in ref.[7]. Response functions have of course since long been the focus of intense studies for the electron gas with numerous contributions. Early works by Lundqvist and Hedin are noticeable leading to the often cited GW method. [8, 9] More recent works include those of Faleev and Stockman focussing on electrons in quantum wells.[10] An alternative method, seemingly simpler than the Bethe-Salpeter, is a real time solution of the Kadanoff Baym two-time equations using conserving approximations of the self-energies. This guarantees that the energy-weighted sum-rule (assuming an effective mass $m^*$)

$$\int_0^\infty \omega S(\omega, q_0) d\omega = \frac{q_0^2}{2m^*}$$

is satisfied. This method was first used by Kwong and Bonitz for the plasma oscillations in an electron gas. [11] The details of this method were already presented in the paper by Kwong and Bonitz. We use it here to calculate response functions in symmetric nuclear matter, emphasizing the relative ease of these computations and also the relation of these calculations to the nuclear many-body problem in general.

The relevant KB-equations, already presented in ref. [11] are shown in the following section followed in section 2.1 by an exposé and explanation of the interactions used at the separate level of approximations. When the system initially correlates with the total energy being conserved, the potential energy of interactions decreases and the kinetic energy increases, i.e. the temperature increases. Section 2.2 shows how to calculate the resulting temperature at equilibrium. Results are shown in section 3. The relation of of our work to the Landau quasi-particle theory is addressed in section 4 and section 5 contains a summary of our results and some conclusions.

2. The two-time KB-equations

The Kadanoff-Baym equations in the two-time form for the specific problem at hand was already shown in previous work, where it was applied to the electron gas in a linear response calculation.[11] Some modifications (related to the difference in interactions and self-energies) are necessary for the present nuclear problem. Correlations are included by defining self-energies in a second order Born approximation with a residual interaction defined by eq.(16) below. This is in addition to a first order mean (Hartree-Fock) field. This then is a ‘conserving approximation’ [5] a necessary requirement when applying the two-time formalism consistently. We compare our results with calculations where correlations are neglected with only the mean field included, the ‘HF+RPA’ approximation. As made clear in ref. [11] there is no need to separately calculate vertex corrections when applying the two-time formalism. It is a major obstacle in using the Bethe-Salpeter formalism. The proper vertex corrections are in our method generated by the time-evolution of the Green’s functions when subjected to the external disturbance. We separate the Green’s function into a spatially homogeneous part $G_{00}$ and a linear response part $G_{10}$.

Calculations proceed as follows: Equilibrium Green’s functions are first constructed for an uncorrelated fermi distribution of specified density and temperature. The $G_{00}$ functions are then time-evolved (for typically $10 fm/c$) with the chosen mean field and correlations until stationary. An external field $U(q,t) = U_0(t)\delta_{q,q_0}$ is then applied which generates particle-hole Green’s functions $G_{10}^\geq$ that propagate in time according to equations already shown in ref. [11] and for completeness repeated here. (Summation over $m = 0, 1$ and integration over $t$ from $-\infty$ to $+\infty$ is implied).
\[
\left(i\hbar \frac{\partial}{\partial t} - \epsilon_k + q_0\right) G_{10}^< (ktt') = U_0(t) G_{00}^> (ktt') + \Sigma_{1m}^{HF} (kt) G_{m0}^>(ktt') + \Sigma_{1m}^R (kt\bar{t}) G_{m0}^A (k\bar{t}t') + \Sigma_{1m}^> (k\bar{t}t') G_{m0}^A (k\bar{t}t')
\]

and
\[
\left(-i\hbar \frac{\partial}{\partial t'} - \epsilon_k\right) G_{10}^> (ktt') = U_0(t') G_{11}^> (ktt') + G_{10}^> (ktt') \Sigma_{m0}^{HF} (kt) + G_{10}^> (k\bar{t}t') \Sigma_{m0}^A (k\bar{t}t') + G_{10}^> (k\bar{t}t') \Sigma_{m0}^A (k\bar{t}t')
\]

Retarded and advanced parts are given by
\[
\Sigma_{nm}^{R/A} (p, t, t') = \pm \theta(\pm (t - t')) \left[ \Sigma_{nm}^> (p, t, t') - \Sigma_{nm}^< (p, t, t') \right]
\]

\[
G_{nm}^{R/A} (p, t, t') = \pm \theta(\pm (t - t')) \left[ G_{nm}^> (p, t, t') - G_{nm}^< (p, t, t') \right]
\]

For the Hartree-Fock self-energy in the (00)-channel we choose a parametrisation shown in section 2.1. The Hartree-Fock self-energy in the (10)-channel is given by
\[
\Sigma_{10}^{HF} (p, t) = -i V_a (q_0) \sum_{p'} G_{10}^< (p', t, t) + \sum_{p'} G_{10}^> (p - p', t, t) V_a (p)
\]

with \( V_a \) specified below in section 2.1. Selfenergies \( \Sigma_{00}^> \) are given by
\[
\Sigma_{00}^> (k, t, t') = i \sum_p G_{00}^> (k - p, t, t') V_s^> (p, t, t').
\]

with
\[
V_s^> (p, t, t') = V^2 (p) \Pi_{00}^> (p, t, t')
\]

where \( V(p) \) is the momentum-representation of the residual potential, local in coordinate space, eq. (16). The polarisation bubble \( \Pi_{00} \) is defined by
\[
\Pi_{00}^> (p, t, t') = -i \sum_{p'} G_{10}^> (p', t, t') G_{00}^> (p - p', t, t)
\]

The selfenergies in the (10) channel are given by
\[
\Sigma_{10}^> (k, t, t') = i \sum_p \left[ G_{10}^> (k - p, t, t') V_s^> (p, t, t') + G_{00}^> (k - p, t, t') V_{s(10)}^> (p, t, t') \right]
\]

where
\[
V_{s(10)}^> (p, t, t') = V_a (p) V_a (p + q_0) \Pi_{10}^> (p, t, t')
\]
Figure 1. Diagrams representing contributions to the self energy in the Kadanoff-Baym equations to zeroth order ($\Sigma_{00}$) and first order ($\Sigma_{10}$) in the external perturbation $U$. The solid (dashed) lines are correlated Green’s functions (NN interactions). The number near each Green’s function line gives the order in $U$ of that line.

and where the potential $V_a$ is defined in section 2.1. The polarisation bubble in the (10)-channel is given by

$$
\Pi_{10}^{\uparrow\downarrow}(p, t, t') = -i \sum_{p'} [G_{10}^{\uparrow\downarrow}(p', t, t')G_{00}^{\uparrow\downarrow}(p' - p, t', t) + G_{00}^{\uparrow\downarrow}(p', t, t')G_{10}^{\uparrow\downarrow}(p' - p - q_0, t', t)]
$$

A diagrammatic representation of the self-energy is shown in Fig. 1.

The eqs. (2) and (3) are time-evolved and the response-function is, after a fourier-transformation of

$$
\delta n(q_0, t) = -i \sum_p G_{10}^{\uparrow\downarrow}(p, t, t)
$$

with respect to time $t$, obtained from

$$
S(\omega, q_0) = \frac{\delta n(q_0, \omega)}{\pi n_0 U_0(\omega)}
$$

2.1. Interactions

The nuclear two-body interaction in ‘free space’ involves a combination of long-ranged one-pion exchange contributions and complicated strong short-ranged attractions and repulsions. This leads to even more complicated ‘in-medium’ interactions and strong correlations in the nuclear many-body environment. Simplifications are necessary to make the exploratory calculations presented here reasonably short. The nuclear model adopted in most similar works is that of nucleons moving in a mean (‘Hartree-Fock self-consistent’) field with mutual in-medium (‘residual’) two-body interaction (potential). A reasonable form of this potential could be a Skyrme (as used in ref. [12]) or the Gogny-interaction (as used in ref. [13]) or some similar
interaction. Apart from these in-medium effective potentials, a semi-realistic NN-interaction with a hard core was used in a Jastrow-correlated extension of the RPA. We are taking a somewhat different approach here adopting three different potentials (I, II and III) each representing different aspects (domains) of the interaction that for the purpose of presentation we assume to be a Brueckner state-independent reaction matrix \( <k|K|k'> \) or \( K(p,q) \) with \( q = k - k' \) and \( p = \frac{1}{2}(k + k') \).

I. An important feature of the Hartee-Fock mean field is that it is momentum-dependent and only the diagonal matrix-elements \( K(p,0) \) are needed. We adopt a parametrisation due to Welke et al\[15\] leading to:

\[
\Sigma^{HF}_{00}(p,t) = A \frac{\rho}{\rho_0} + B \left( \frac{\rho}{\rho_0} \right)^\sigma + 2C \int \frac{n(p',t)}{1 + (p'-p)^2/(2\pi)^3} dp'
\]

(14)

with \( A = -110.44 \) MeV, \( B = 140.9 \) MeV, \( C = -64.95 \) MeV, while \( \rho \) is the density of the symmetric nuclear matter under consideration and \( \rho_0 \) the saturation density. The momentum-distribution function \( n(p,t) \) is defined below.

We shall also, in separate calculations substitute this mean field by assuming an effective mass.

II. To calculate the second order Born diagrams we need off-diagonal matrix-elements of the interaction i.e. its \( q \)-dependence. We choose here an interaction often used in this context, first introduced by Danielewicz [16, 6, 7, 17] and given by:

\[
V(r) = V_0 e^{-\frac{r^2}{\eta^2}}
\]

(15)

with \( \eta = 0.57fm \) and \( V_0 = -453 \) MeV.

In momentum-space it reads:

\[
V(q) = \pi^{3/2} \eta^3 V_0 e^{-\frac{1}{4}q^2\eta^2}
\]

(16)

We use this interaction to calculate self-energies \( \Sigma_{00}^\sigma \) and \( \Sigma_{00}^\rho \).

III. The linear response calculation involves excitations near the fermi-surface i.e. matrix-elements \( K(q,p \sim p_F) \) for which the \( p \)-independent interaction (16) is too strong, leading to divergences if used for calculating the (10) field components. This is related to a too large numerical value for the Landau parameter. Numerical results shown below are therefore made with an interaction \( V_\sigma(q) = a_{10} V(q) \) used in the calculation of \( \Sigma_{10} \). The majority of the calculations presented below are with \( a_{10} = 0.3 \). Other values are chosen below together with a discussion of the Landau parameter. (See section 4.)

2.2. Equilibrium Temperature

In a KB-calculation with selfenergies defined in a conserving approximation the total energy is conserved; the potential energy decreases and kinetic energy increases with the same amount until internal equilibrium. The result is an increase in temperature from the initially set value. This situation can be moderated by an imaginary time-stepping method [16, 17, 18]. The final temperature \( T_f \) will be a function of the initial imaginary time \( \tau \) (and initial temperature) with \( T_f \rightarrow 0 \) in the limit \( \tau \rightarrow \infty \).

For finite values of \( \tau \) this final equilibrium temperature \( T_f = 1/\beta \) and chemical potential \( \mu \) are related to the equilibrium self-energies \( \Sigma^< \) and \( \Sigma^> \) by [19]:

\[
\Sigma^>(p,\omega) = -e^{\beta(\omega - \mu)} \Sigma^<(p,\omega).
\]

(17)

(The ratio of the selfenergies is consequently independent of momentum \( p \), which serves as a check on numerical accuracy.)
With $\beta$ and $\mu$ calculated from eq. (17) the equilibrium uncorrelated distribution function is given by

$$f(p) = 1/(1 + e^{\beta(\omega(p) - \mu)})$$

with

$$\omega(p) = \frac{p^2}{2m} + Re\Sigma^+(p, \omega) + \Sigma^{HF}_{00}(p)$$

The real part of $\Sigma^+$ is calculated from the imaginary part by the dispersion relation, and using the relation

$$2Im\Sigma(p, \omega) = i(\Sigma^<(p, \omega) - \Sigma^>(p, \omega))$$

While the uncorrelated distribution is given by eq. (18) the correlated one is given by

$$n(p, t) = -iG^<(p, t, t).$$

3. Numerical results

Calculations are made for symmetric nuclear matter at normal nuclear matter density; $\rho = 0.13$fm$^{-3}$, i.e. fermi-momentum $k_F = 1.25$fm$^{-1}$. The external momentum transfer is chosen to be either $q_0 = 0.2, 0.4$ or $0.8$fm$^{-1}$. The calculations follow essentially the computing-methods described in ref.[20] with the additional requirement to also time-evolve $G_{10}$.

All numerical results shown below are without the initial imaginary time-stepping. The initial ($t=t'=0$) distribution $n(p, 0) = G_{00}^<(p, 0, 0)$ is taken to be a zero temperature fermi-distribution except in the uncorrelated case where $T = 5$ MeV. The system is then time-evolved and correlations are completed at $t \geq t_c$ after which time the distribution $n(p)$ is stationary. In the linear response evolution used here, separating the Green's function into $G_{00}$ and $G_{10}$ components, the collision term for $G_{00}(p, t, t)$ evolution will vanish for $t > t_c$. (See ref. [18] for a detailed discussion of correlation times $t_c$.)

Fig. 2 shows the relevant distribution-functions. Solid curves show the initial zero-temperature Fermi-distribution and the correlated distribution. The temperature obtained as described above was 5 MeV. The dotted curve in Fig. 2 shows the Fermi-distribution for this temperature. With the correlations completed in the (00) channel the external field $U_0(t)$ is now applied generating the $G_{10}$ field as shown by eqs. (2) and (3). Note that with the conserving approximation satisfied the vertex-correction is 'automatically' included in the ensuing time-evolution.[11]
The resulting time dependent density

\[ \delta n(q_0, t) = -i \sum_p G_{10}^< (p, t, t) \]

is recorded until it is fully damped. If the damping time is too large (number of time-steps \( > \sim 150 \)) then \( n(q_0, t) \) is extrapolated using the amplitudes and frequencies of the oscillations for lesser times. A typical result of the evolution in real time is shown in Fig. 3. This time-function is then fourier-transformed to \( \omega \)-space to obtain linear response functions \( S(\omega, q_0) \). Results are shown in Fig. 4 for three different external momenta transfers \( q_0 \). The solid lines show the results including correlations while the broken lines show the uncorrelated (‘HF+RPA’) results. These latter results are obtained using a temperature \( T = 5 \text{MeV} \) obtained from eq. 17. They are in overall agreement with previous RPA calculations e.g. [12, 13, 7]. There are some differences to be expected because of the variety of two-body interactions and mean fields that have been used. The heating to \( T = 5 \text{MeV} \) causes only a very slight broadening in comparison with a \( T = 0 \) calculation.

As regards the correlated results (the solid lines) , the initial temperature at time \( t = 0 \) is, as already stated above, equal to zero; the momentum-distribution is that of a zero-temperature fermi-distribution. The correlations result in a heating to \( T = 5 \text{MeV} \) and an associated smoothing of the fermi-surface. An additional and more significant smoothing is due to the broadening of the static spectral-functions in the correlated medium. There is also a considerable depletion of the distribution at low momenta caused by the correlations.(See Fig. 2) This is the most probable cause for the difference between the correlated and uncorrelated cases in the
region of the large values of frequencies $\omega$. Other than that there is in fact no other major effect of the correlations.

In order to show the approach to equilibrium in some detail the density $iG^<_{10}(p,t,t)$ is integrated over $p_x$ and $p_y$ ($p_z$ being the component along $q_0$). The resulting $t$ and $p_z$ dependent function is shown in Fig. 5 for the correlated case.

It shows that the excitations take place close to the fermi-surface where the quasi-particle picture dominates and where spectral functions have a vanishing width. The correlations affect mainly the deeper lying states. This fact serves to explain the relatively small effect of the correlations, other than at the high frequency end of the response functions. This situation may however not be the case for tensor correlations [21], that have a longer range (in coordinate-space) and not included here.

The results in this section were all obtained with the factor $a_{10} = 0.3$. Fig. 6 below, also shows response functions for $a_{10} = 0.4, 0.3$ and $0.1$ and with an effective mass $m^* = 0.7$ in lieu of the mean field eq. 14.

4. Landau parameters
Owing to the relatively low temperature and long fluctuation wavelengths considered here, the excitations in our linear response calculations are concentrated around the fermi-surface. This is clearly evident from Fig. 5 which, as pointed out above, can explain why the NN-collisions have a smaller effect than might be expected. This is also why Landau-theory is applicable here. Another related reason why this theory is pertinent to our work is the well known relation [22] between the Landau-parameter

$$F_0 = \frac{2m^*k_F}{2\pi^2\hbar^2}f_0$$

(22)

and the ring-diagram correlations, the collective excitation we are dealing with here. The factor $f_0$ is here the angular momentum ($l = 0$) quasi-particle (effective) interaction. The Landau parameter relates to the compressibility $K$ by

$$K = 6e_F(1 + F_0)$$

(23)

with $e_F$ being the Fermi energy. The interaction $f_0$ is composed of a 'direct' part defined by the functional derivative

$$f_{kk'} = \frac{\partial^2 E}{\partial n_k n_{k'}}$$

(24)

(with $k \rightarrow k'$) and an 'induced' part. The 'induced' interaction is essentially the effect of screening by rings and further defined below.
Figure 6. Solid curves show response functions $S(\omega, q_0)$ with second order self-energies for $q_0 = 0.4\text{fm}^{-1}$ and Landau parameters $F_0^{(d)} = -0.799, -0.599$ and $-0.200$ ($a_{10} = .3, .4$ and $0.1$, respectively), from left to right. An effective mass $m^* = 0.7$ was assumed. [15]

Guided by methods used by Babu and Brown[22], who considered interactions in liquid $^3$He, Sjöberg [23] and later others (see e.g. ref. [26]) calculated Landau parameters for nuclear matter. They used Brueckner’s $K$-matrix expression for the total energy $E$ in the analysis. The 'direct' interaction is then just the Brueckner $K$-matrix while the 'induced', $f_i$ is of higher orders of $K$. They find that it is defined by

$$ f_i(k, k) = -\sum_{p, p'} f(k, p) \left( \frac{\delta n_p(q, \omega)}{\delta U_{p'}(q, \omega)} \right)_{q, 0} f(p', k) $$

(25)

Note that the perturbative potential $U_{p'}$ is here assumed to act on particles of momenta $p'$ only, to generate density fluctuation $\delta n_p$. Our interactions are not 'realistic' enough to warrant a detailed comparison with Sjöberg’s (or other’s based on Brueckner theory). It is here made only to illustrate the connection of our work with that based on Brueckner theory.[22, 23] From the result of the calculation of response function shown in Fig. 4 (2nd order correlations) for $a_{10} = .3$ and for $q = 0.2\text{fm}^{-1}$ we find $\frac{\delta n}{\delta U} = .00126$ to get for the 'induced' interaction 24 MeV with the 'direct' being 140 MeV to get $F_0 = -0.495$ to compare with Sjöberg’s $F_0 = -0.373$.

Landau theory is a quasi-particle theory and applies to the limit $q = 0$ which is not attainable in our method of calculation. Furthermore, our calculation goes beyond the quasi-particle. The strength of the interaction, our factor $a_{10}$, does of course also affect the result. Fig. 6 shows the dependence of the the response on this strength-factor. The values of the Landau parameters $F_0^{(d)}$ are in this figure calculated using only the 'direct' interactions.

5. Summary and Conclusions

The main purpose of this presentation is to illustrate the usefulness of the two-time Green’s function (Kadanoff-Baym) method for the study of nuclear response. It was previously applied to the electron gas to see the effect of correlations.[11] The time-evolution of Green’s function in two-time space with conserving approximations for the self-energies guarantees the preservation of sum-rules. An alternative method, the solution of the Bethe-Salpeter (BS) equation (in $\omega$-space) was been carried out by Bozek et al.[6, 7].

The rise in temperature associated with the onset of correlations when using the two-time method is sometimes cited as a drawback. It is however not difficult to remedy by allowing the correlations to initially form by propagating along the imaginary time-axis. It requires of course to have access to the proper computer-codes. It is our aim to utilise our existing codes in future work.

Our calculations show some differences between the two approximations (collisionless and


but mainly at the high frequency end of the response functions. This is accompanied by a corresponding difference in peak energies, but without any significant shift of these energies. The results shown are for symmetric nuclear matter. Response calculations for neutron matter is of particular interest related to astrophysical problems, in particular neutrino-absorption.

One reason for choosing a local potential (eq. 15) as done here is that the 2-time computer-code ([20]) used here is restricted to this choice although in-medium effective interactions are known to be non-local. Separable interactions have been obtained from inverse scattering [25] and these can now be used in a new 2-time code developed specifically for these separable (i.e. non-local) potentials.

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