Solid State Communications 149 (2009) 476–480

Contents lists available at ScienceDirect

Solid State Communications

journal homepage: www.elsevier.com/locate/ssc

Multiquantum kinetic equation and charge density fluctuations

A.A. Klyukanov *

State University of Moldova, Department of Physics, Kishinau, 2009, Mateevici 60, Republic of Moldova

ARTICLE INFO

Article history:
Received 3 December 2008
Received in revised form
16 December 2008
Accepted 17 December 2008
by A.H. MacDonald
Available online 25 December 2008

PACS:
71.10.-w
71.45.-d
72.10.Bg

Keywords:
A. Metals
D. Exchange
D. Electron–electron interactions
D. Fluctuations

ABSTRACT

A multiquantum integral equation for the longitudinal dielectric function is derived accounting for of pair correlations. The Heisenberg equation of motion and fluctuation-dissipation theorem has been used to calculate a microscopic polarization. It has been shown that a kinetic equation for a polarization may be represented as a power series in fluctuations of instantaneous field near the mean field. Direct Coulomb pair correlations have been evaluated explicitly by means of a fluctuation-dissipation theorem. The energy and the effective mass of an electron of momentum k in the degenerate electron system and damping of one-electron states have been computed at $r_s \geq 1$.

© 2009 Elsevier Ltd. All rights reserved.

1. General consideration

Correlation effects influencing the kinetic properties of semiconductors [1–3] and metals [4–6] are intensively studied at the present time. Processes of photon emission and absorption with simultaneous creation of a few optical plasmons as typical electronic eigenmodes induced by charge carriers correlations were investigated experimentally and theoretically [1–3].

Physical properties of transition metals, correlation energy, lifetimes of electrons, non-Fermi-liquid behavior and Cooper pair formation have been investigated in [4–6].

In spite of the fact that all of these investigations [1–6] quite naturally deal themselves, from the outset, with different correlation effects, the theoretical approaches derived have some common features. First of all there is a standard non-relativistic many-body Hamiltonian given by the expression:

$$\hat{H} = \sum_{\alpha,n,m} h^{\alpha}_{nm}\hat{a}^{+}_{n\alpha}\hat{a}_{m\alpha} + \frac{1}{2}\sum_{q,\alpha} V^{\alpha\alpha}_{q} \sum_{m,n,l,p} \mathrm{e}^{\mathrm{i}qr_{\alpha}}_{l,n}\mathrm{e}^{-\mathrm{i}qr_{\alpha}}_{p,m}\hat{a}^{+}_{l\alpha}\hat{a}^{+}_{p\alpha}\hat{a}_{m\alpha}\hat{a}_{n\alpha}, \quad (1)$$

$$V^{\alpha\beta}_{q} = \frac{4\pi \mathrm{e}_{\alpha}\mathrm{e}_{\beta}}{Vq^2},$$

where $V^{\alpha\beta}_{q}$ is the Fourier transform of Coulomb potential, $\hat{a}^{+}_{i\alpha}$, $\hat{a}_{f\alpha}$ are the creation and destruction operators, n — collective index, incorporated all the degrees of freedom. The l, p, m, n subscripts represent the quantum numbers sets, describing the system of one-particle eigen-states. The $\alpha = e, n$ index distinguishes electrons and nuclei. The last term in Eq. (1) describes the repulsive Coulomb interaction among electrons $\alpha = e$ and among nuclei $\alpha = n$. The matrix $h^{\alpha}_{n,m}$ parameterises operator

$$\hat{h}^{\alpha} = \frac{1}{2m_{\alpha}}\left(\hat{p}_{\alpha} - \frac{\mathrm{e}_{\alpha}}{c}\hat{A}_{\alpha}(r_{\alpha}, t)\right)^2 + \mathrm{e}_{\alpha}\,\varphi\,(r_{\alpha}, t) + \sum_{\beta}^{\alpha}\sum_{q} V^{\alpha,\beta}_{q}\mathrm{e}^{\mathrm{i}qr_{\alpha}}\hat{\rho}^{\beta}_{q}$$

$$\hat{\rho}^{\beta}_{q} = \sum_{n,m} \mathrm{e}^{-\mathrm{i}qr_{\beta}}_{nm}\hat{P}^{\beta}_{nm}, \qquad \hat{P}^{\alpha}_{nm} = \hat{a}^{+}_{n\alpha}\hat{a}_{m\alpha}. \quad (2)$$

Here $\hat{p}_{\alpha}$ is the momentum operator, r_{α} is the radius vector of particle with charge e_{α}. The symbol α at sum after β means that the term with $\beta = \alpha$ have to be excluded. Other designations are standard.

The lagging response of a many-body system with Hamiltonian (1) to the external longitudinal and transversal electromagnetic fields perturbations, the charge density and the macroscopic polarization are determined by the operator of microscopic polarization $\hat{P}^{\alpha}_{if}$ time dependence [1–5]. Thus, the problem reduces to determination of expectation value

* Fax: +373 22 24 42 48.
E-mail address: klukanov@cinf.usm.md.

0038-1098/$ – see front matter © 2009 Elsevier Ltd. All rights reserved.
doi:10.1016/j.ssc.2008.12.033

$$P^{\alpha}_{if}(t) = \langle \hat{P}^{\alpha}_{if}(t)\rangle, \qquad \langle \hat{A}(t)\rangle = Sp\{\hat{\rho}_0 \hat{A}(t)\},$$
$$\hat{A}(t) = \hat{U}^{+}(t)\hat{A}\hat{U}(t), \qquad \hat{U}(t) = T\exp\left(-\frac{\mathrm{i}}{\hbar}\int_0^t H(s)\mathrm{d}s\right), \tag{3}$$

where $U(t)$ is the evolution operator. Angular brackets denote averaging with the equilibrium density operator. In terms of creation and destruction operators according to the formula (2) the time dependence of the polarization operator $\hat{P}^{\alpha}_{if}$, has to be *ab initio* derived from the Heisenberg equation of motion. Working out commutators, one obtains

$$\begin{aligned}\frac{\hbar}{\mathrm{i}}\frac{\partial P^{\alpha}_{if}}{\partial t} &= \frac{\hbar}{\mathrm{i}}\dot{P}^{\alpha}_{if} = \sum_n (h_{ni}P^{\alpha}_{nf} - P^{\alpha}_{in}h_{fn}) \\ &+ \sum_q V^{\alpha\alpha}_q \sum_{m,n,l} (\mathrm{e}^{\mathrm{i}qr_\alpha}_{ln}\mathrm{e}^{-\mathrm{i}qr_\alpha}_{fm}\langle \hat{a}^{+}_{l\alpha}\hat{a}^{+}_{i\alpha}\hat{a}_{n\alpha}\hat{a}_{m\alpha}\rangle \\ &- \mathrm{e}^{\mathrm{i}qr_\alpha}_{li}\mathrm{e}^{-\mathrm{i}qr_\alpha}_{nm}\langle \hat{a}^{+}_{n\alpha}\hat{a}^{+}_{l\alpha}\hat{a}_{m\alpha}\hat{a}_{f\alpha}\rangle).\end{aligned} \tag{4}$$

The second part of Eq. (4) shows contributions due to correlated four-operator terms. The dynamical Hartree–Fock (HF) like approximation according to which

$$\begin{aligned}\langle \hat{a}^{+}_l\hat{a}^{+}_i\hat{a}_n\hat{a}_m\rangle &= \langle \hat{a}^{+}_l\hat{a}_m\rangle\langle \hat{a}^{+}_i\hat{a}_n\rangle - \langle \hat{a}^{+}_l\hat{a}_n\rangle\langle \hat{a}^{+}_i\hat{a}_m\rangle \\ &= P_{lm}P_{in} - P_{ln}P_{lm}\end{aligned} \tag{5}$$

provides what is believed to be a simplest approximation for the solution of the many-body problem with Hamiltonian (1), (index α is temporarily omitted). This way one obtains the well-known Bloch equation. It is necessary to note that in all above-mentioned different theories [1–6] the HF approximation is used as the starting point. The HF factorization (5) yields a result for microscopic polarization $P_{if}(t)$

$$\begin{aligned}&\frac{\hbar}{\mathrm{i}}\dot{P}^{HF}_{if}(t_1) = \left\langle\left[\hat{H}', \hat{P}_{if}(t)\right]\right\rangle \\ &= \hbar\omega^{HF}_{if}(t)P_{if}(t) + \sum_n^i \tilde{h}^{if}_{ni}(t)P_{nf}(t) - \sum_n^f \tilde{h}^{if}_{fn}(t)P_{in}(t),\end{aligned}$$

$$\hbar\omega^{HF}_{if} = \tilde{h}_{ii} - \tilde{h}_{ff} + \sum_n^f M^{ff}_{in}P_{in} - \sum_n^f M^{ii}_{nf}P_{nf}. \tag{6}$$

This equation is mathematically identical to the Schrodinger equation with mean-field Hamiltonian

$$\begin{aligned}&\hat{H}' = \sum_{n,m}\tilde{h}_{nm}\hat{a}^{+}_n\hat{a}_m, \quad \tilde{h}_{nm} = h_{nm} + \sum_{l,p}M^{lp}_{nm}P_{lp}, \\ &M^{lp}_{nm} = \sum_q V_q(\mathrm{e}^{\mathrm{i}qr}_{nm}\mathrm{e}^{-\mathrm{i}qr}_{lp} - \mathrm{e}^{\mathrm{i}qr}_{np}\mathrm{e}^{-\mathrm{i}qr}_{lm}), \qquad \tilde{h}^{if}_{nm} = \tilde{h}_{nm} - M^{if}_{nm}P_{if}.\end{aligned} \tag{7}$$

Eq. (6) has to be considered a definition of the generalized transition frequency $\hbar\omega^{HF}_{if}(t)$. Besides the Hartree–Fock difference of proper energies $\tilde{h}_{ii} - \tilde{h}_{ff}$ of initial i and final f states (Koopmans approximation), Eq. (6) takes into account the unscreened exciton Coulomb interaction between the quasi-particle in f state and quasi-hole in i state.

As is known, the random phase approximation supposes the replacement of instantaneous field created by plasma with mean field [5,7]. The microscopic polarization, calculated in the mean-field HF approximation (6), can be used next for evaluation of the response function, the light absorption coefficient, the spontaneous recombination rate and so on [1–7]. It leads to important consequences for the kinetic properties of solid states [5, 7]. Eq. (6) at the level of dynamical HF approximation allow to including the generalized random phase approximation into the consideration [5,7,8].

There are no difficulties in deriving an Eq. (6) with the use of the HF decoupling scheme (5) but it is much more difficult to establish the validity of such a procedure This work pursues two goals. First, to carry out *ab initio* derivation of multiquantum kinetic equation with a special emphasis on the many-body correlations. In particular, we calculate the dielectric function $\varepsilon(q,\omega)$ with account of fluctuations near the mean field in Eq. (4). Second, our aim is to calculate the energy and the effective mass of an electron of momentum k in the degenerate electron system and damping of one-electron states at $r_s \geq 1$ (r_s is the unit-sphere radius in Bohr radii).

2. Multiquantum kinetic equation

To study the correlation contributions to kinetic equation Eq. (4) one has to go beyond the mean-field HF approximation (6). To extend the theory beyond the HF level we start by considering the deviations of the exact terms from their corresponding HF factorized parts

$$\dot{P}_{if}(t) = \dot{P}^{HF}_{if}(t) + \dot{P}^{C}_{if}(t). \tag{8}$$

The quantity $\dot{P}^{C}_{if}(t)$ is defined as correlation part of kinetic equation for microscopic polarization. There are some interesting properties of it. First, the Hartree–Fock factorization scheme (5) is explicit in the quasi-particle picture. Thus, first remarkable feature of Eq. (8) is that in the quasi-particle picture ($\hat{H} \to \hat{H}_q$) the correlation part is identically zero

$$\dot{P}^{qC}_{if}(t) = 0, \qquad \hat{P}^{q}_{if}(t) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\hat{H}_q t}\hat{P}_{if}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}_q t}, \qquad \hat{H}_q = \sum_{n\alpha}E_{n\alpha}\hat{P}^{\alpha}_{nn}. \tag{9}$$

Another feature appears if one calculates the correlation part $\dot{P}^{C}_{if}(t)$ (8) by means of the approximation, according to which only term $T\exp(\frac{\mathrm{i}}{\hbar}\int_s^t \hat{V}(s_1)\mathrm{d}s_1)$ in the exact expression for operator of evolution

$$\begin{aligned}&U(t) = \exp\left(-\frac{\mathrm{i}}{\hbar}\hat{H}_q t\right) - \frac{\mathrm{i}}{\hbar}U(t)\int_0^t T\exp\left(\frac{\mathrm{i}}{\hbar}\int_s^t \hat{V}(s_1)\mathrm{d}s_1\right)\hat{V}(s)\mathrm{d}s, \\ &\hat{V} = \hat{H} - \hat{H}_q\end{aligned} \tag{10}$$

may be expanded as power series in $\hat{V} = \hat{H} - \hat{H}_q$. Keeping the first order terms to develop the equation of motion for microscopic polarization with account of correlation part $\dot{P}^{C}_{if}(t)$ we obtain for arbitrary operator $\hat{P}(t)$ the result

$$\begin{aligned}&\hat{P}(t) = \hat{P}_q(t) + \frac{\mathrm{i}}{\hbar}\int_0^t \left\langle[\hat{V}(t_1), \hat{P}(t)]\right\rangle \mathrm{d}t_1, \\ &\hat{V}(t) = U^{+}(t)\hat{V}U(t).\end{aligned} \tag{11}$$

Thus, the correlation part $\dot{P}^{C}_{if}(t)$ takes the form

$$\begin{aligned}\dot{P}^{C}_{if}(t) &= \frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}t_1 \Bigg\{\langle[\hat{V}(t_1), \hat{P}_{if}(t)]\rangle \\ &- \frac{\mathrm{i}}{\hbar}\sum_{n,m}(\langle[\hat{V}(t_1), \hat{\tilde{h}}_{nm}(t)]\rangle\langle[\hat{P}_{nm}(t), \hat{P}_{if}(t)]\rangle \\ &+ \tilde{h}_{nm}(t)\langle[\hat{V}(t_1), [\hat{P}_{nm}(t), \hat{P}_{if}(t)]]\rangle)\Bigg\}.\end{aligned} \tag{12}$$

Eq. (12) for $\dot{P}^{C}_{if}(t)$ can be further simplified by carrying out partial decoupling. In terms of fluctuations of instantaneous field near the mean field this approximate expression for correlation part may be written as

$$\begin{aligned}&\dot{P}^{C}_{if}(t_1) = \frac{1}{\hbar^2}\int_0^{t_1}\mathrm{d}t_2\,\{I(1,2) - I(2,1)\}, \\ &I(1,2) = \sum_{n_1m_1}\sum_{n_2m_2}\langle\Delta\hat{h}_{n_1m_1}(t_1)\Delta\hat{\tilde{h}}_{n_2m_2}(t_2)\rangle\langle\Delta[\hat{P}_{n_1m_1}(t_1), \\ &\hat{P}_{if}(t_1)]\Delta\hat{P}_{n_2m_2}(t_2)\rangle, \quad \Delta\hat{P} = \hat{P} - \langle\hat{P}\rangle\end{aligned} \tag{13}$$

where fluctuations near mean field are determined by equations

$$\Delta\hat{h}_{nm}(t) = \sum_q \sum_\beta V_q^{\alpha\beta} \mathrm{e}^{\mathrm{i}qr_\alpha}_{nm} (\hat{\rho}_q^\beta(t) - \langle\hat{\rho}_q^\beta(t)\rangle),$$
$$\Delta\hat{\tilde{h}}_{nm}(t) = \Delta\hat{h}_{nm}(t) - \sum_q V_q^{\alpha\beta} \mathrm{e}^{\mathrm{i}qr}_{np} \mathrm{e}^{-\mathrm{i}qr}_{lm} (\hat{P}_{lp}(t) - \langle\hat{P}_{lp}(t)\rangle). \quad (14)$$

It is instructive to note here that the deviation of the first order correction (12) and approximate equation (13) in the quasi-particle picture vanishes. Hence, a further remarkable feature of correlation part $\dot{P}^C_{if}(t)$ is that it may be represented as power series in fluctuations $\Delta\hat{h}_{nm}(t)$. Eq. (13) is obtained with account of pair correlations.

Direct Coulomb interaction gives the contribution into the correlator density-density, which is proportional to V_q^2 and diverges as q^{-4} at $q \to 0$, if we restrict the consideration with second order correction of standard perturbation theory. To avoid this difficulty some authors replace the unscreened Coulomb potential by its screened value. But screening should result from the proper treatment of correlations. The expectation value of charge density operator's multiplication $\langle\hat{\rho}_q(t)\hat{\rho}_{-q}(s)\rangle$, taken in different time points in Eq. (14), specifies memory effects. It can be precisely calculated within the fluctuation-dissipation theorem [7] and can be expressed in terms of structure factor or inverse dielectric function

$$\langle\Delta\hat{h}_{n_1m_1}(t_1)\Delta\hat{h}_{n_2m_2}(t_2)\rangle = \frac{\hbar}{\pi}\sum_q V_q \sum_{n_{1,2}m_{1,2}} \mathrm{e}^{\mathrm{i}qr}_{n_1m_1}\mathrm{e}^{-\mathrm{i}qr}_{n_2m_2} \times \int_{-\infty}^{\infty} \exp(-\mathrm{i}\omega(t_1-t_2))[n(\omega)+1]\mathrm{Im}\left\{\frac{1}{\varepsilon^*(\kappa,\omega)}\right\}\mathrm{d}\omega,$$
$$n(\omega) = \left[\exp\left(\frac{\hbar\omega}{k_0T}\right) - 1\right]^{-1}, \quad (15)$$

where asterisk signifies the complex conjugate. The zeroes of dielectric function $\varepsilon(q,\omega)$ determine the frequencies of the quasi-particles interacting with electrons. The using of the fluctuation-dissipation theorem is the simplest way to account for infinite series in V_q. At the level of Markov approximation, where one ignores the memory effect, it can be easily seen that Eq. (15) leads to the well-known Boltzmann collision term. At this stage, we already have a closed set of integral equations (6), (8) and (13)–(15). The correlator density-density from Eq. (15) depends on the longitudinal dielectric function. On the other hand, dielectric function $\varepsilon(q,\omega)$ depends on the microscopic polarization in its turn. Hence, Eqs. (6)–(9), (9) and (11)–(15) constitute a self-consistent set of multi-quantum integral kinetic equations.

By expanding the correlation part up to the third order in $\Delta\hat{h}_{nm}(t)$ we obtain

$$\dot{P}_{if}(t) = \dot{P}^{HF}_{if}(t) + \dot{P}^C_{if}(t) + \delta\dot{P}^C_{if}(t),$$
$$\delta\dot{P}_{if}(t_1) = \left(\frac{\mathrm{i}}{\hbar}\right)^3 \int_0^{t_1}\mathrm{d}t_2\int_0^{t_2}\mathrm{d}t_3\,\{I(1,2,3) - I(2,1,3) - I(3,1,2) + I(3,2,1)\}. \quad (16)$$

Index $i = 1, 2, 3$ is the collective index $i = n_im_i$. The third order in $\Delta\hat{h}_{nm}(t)$ term $I(1,2,3)$ is

$$I(1,2,3) = \sum_{1,2,3}\langle\Delta\hat{h}_1(t_1)\Delta\hat{h}_2(t_2)\Delta\hat{\tilde{h}}_3(t_3)\rangle\langle\Delta[\hat{P}_1(t_1), \hat{P}_{if}(t_1)] \times \Delta\hat{P}_2(t_2)\Delta\hat{P}_3(t_3)\rangle, \quad \Delta\hat{P} = \hat{P} - \langle\hat{P}\rangle. \quad (17)$$

According to determination (3) all terms in Eqs. (11)–(17) contain exact operator $\hat{U}(t)$. Thus, the approximation derived shows that the correlation part may be represented as a power series in fluctuations $\Delta\hat{h}_{nm}(t)$. We take pair correlations of $\Delta\hat{h}_{nm}(t)$ into the consideration. The next section is used to present and discuss several results, which stem from this formulation.

3. Electron correlation energy and damping of one-particle states

In this section, we show examples of the numerical solutions of our microscopic theory. Using the results obtained, we can calculate the longitudinal dielectric function with account of pair correlations (15).

$$\varepsilon(q,\omega) = 1 - \frac{\mathrm{i}}{\hbar}\sum_\alpha V_q^{\alpha\alpha}\sum_{i,f} G_{if}(\omega)\left\{\left|\mathrm{e}^{\mathrm{i}qr}_{if}\right|^2(n_f - n_i) - \frac{\mathrm{i}}{\hbar}\sum_{q_1} V_{q_1}\sum_{i,f,l,p}\mathrm{e}^{\mathrm{i}qr}_{il}\mathrm{e}^{\mathrm{i}q_1r}_{lp}\mathrm{e}^{-\mathrm{i}qr}_{pf}\mathrm{e}^{-\mathrm{i}q_1r}_{fi}(n_l - n_p) \times G_{pl}(\omega)\left[\frac{n_f}{\varepsilon(q_1,\omega+\omega_{pf})} - \frac{n_i}{\varepsilon(q_1,\omega+\omega_{il})}\right]\right\}. \quad (18)$$

Here, at the level of the quasi-particle approximation (self-consistent perturbation theory)

$$G_{if}(\omega) = \int_0^\infty \exp[i(\omega+\mathrm{i}\delta)t]\,G^q_{if}(t)\mathrm{d}t = \frac{\mathrm{i}}{\omega+\omega^q_{if}+\mathrm{i}\delta},$$
$$G^q_{if}(t) = \exp(\mathrm{i}\omega^q_{if}t), \qquad \hbar\omega^q_{if} = E_i - E_f, \quad (19)$$

where δ is the infinitesimal positive quantity. We have included here the Coulomb-exchange contribution (Fock-field) to the polarization field and its fluctuations near mean field. The results of the work [8] can be obtained from Eqs. (18) and (19) if one has calculated the transition frequency ω_{k,k_1} at the level of first order approximation of exchange-interacting electrons $\hbar\omega^{HF}_{k,k_1} = \mathrm{e}_k - \mathrm{e}_{k_1} - \sum_q V_q(n_{k+q} - n_{k_1+q})$, $\mathrm{e}_k = \hbar^2k^2/2m$ and set $\varepsilon(q_1,\omega+\omega_1) = 1$. It is emphasized that Eq. (18) cannot be obtained in the mean field HF theory. Mean-field generalized random phase approximation [8] yields the only expression (18) with $\varepsilon(q_1,\omega+\omega_1) = 1$.

To obtain an additional insight into our equations we turn to the special case, which can be evaluated by a simple approximation $\hat{P}_{n,m}(t_1) = G_{n,m}(t_1,t_2)\hat{P}_{n,m}(t_2)$. Making use of Eqs. (13)–(15) we obtain the generalized transition frequency $\hbar\omega_{if}(t)$ in the form

$$\hbar\omega_{if}(t) = \hbar\omega^{HF}_{if}(t) + \Delta E^f_i(t) - \Delta E^{i^*}_f(t)$$
$$\Delta E^f_i(t) = \frac{\mathrm{i}}{\pi}\sum_q V_q\int_{-\infty}^\infty \mathrm{d}\omega[n(\omega)+1]\mathrm{Im}\left\{\frac{1}{\varepsilon^*(q,\omega)}\right\} \times \int_0^t\left(\sum_n\left|\mathrm{e}^{\mathrm{i}qr}_{in}\right|^2 G_{ni}(t,t_1)\varphi^\omega_n(t-t_1) - \mathrm{e}^{\mathrm{i}qr}_{ii}\mathrm{e}^{-\mathrm{i}qr}_{ff}\varphi^\omega_i(t-t_1)\right)\mathrm{d}t_1 \quad (20)$$
$$\varphi^\omega_n(t-t_1) = n_n\exp(-\mathrm{i}\omega(t-t_1)) + (1-n_n)\exp(\mathrm{i}\omega(t-t_1)).$$

The last excitonic term from Eq. (16) which is proportional to $\mathrm{e}^{\mathrm{i}qr}_{ii}\mathrm{e}^{-\mathrm{i}qr}_{ff}$ can be reduced by carrying out the time and frequency integration with using the equation

$$\frac{1}{\pi}\int_{-\infty}^\infty \mathrm{d}\omega[n(\omega)+1]\mathrm{Im}\left\{\frac{1}{\varepsilon^*(q,\omega)}\right\}\left\{\frac{1}{\omega-\omega_1}+\frac{1}{\omega+\omega_1}\right\} = 1 - \frac{1}{\varepsilon(q,\omega_1)}. \quad (21)$$

This equation at $\omega_1 = 0$ shows that direct excitonic Coulomb interaction of the electron and the hole is screened statically. On the other hand, the exchange interaction is exposed to dynamical screening. It can be easily shown by using the quasi-particle approximation $G_{ni}(t,t_1) = \exp(\mathrm{i}\omega^q_{ni}(t-t_1))$, $n = f$ and Eq. (21).

The dynamical screening of the correlation contribution in the energy of quasi-particles is taken into account. The results of the

work [9] obtained by Green function method can be evaluated from Eq. (20) if one takes random phase approximation for dielectric function. More than that, the Coulomb interaction leads to the multiquantum transition processes studied in the works [1–3].

At the high energies $E \approx E_F$, where E_F is the Fermi energy, valence electrons do not "feel" the periodical potential of the solid state and can be considered as practically free. Using the quasi-particle approximation for $G_{ni}(t) = \exp(i\omega_{ni}^{q} t)$ and integrating over time yields

$$E_k(t) = e_k - \sum_q V_q n_{k+q} + E_k^C(t). \tag{22}$$

The contribution of correlation, which will be designated by index C, is defined by the equation

$$E_k^C(t) = \frac{1}{\pi}\sum_q V_q \int_{-\infty}^{\infty} d\omega [n(\omega)+1] \mathrm{Im}\left\{\frac{1}{\varepsilon^*(q,\omega)}\right\} \times \left\{(1-n_{k+q})\Phi(t,\omega_{k,k+q}-\omega) + n_{k+q}\Phi(t,\omega_{k,k+q}+\omega)\right\}, \tag{23}$$

where functions $\Phi(t,\Omega)$ are determined as

$$\Phi(t,\Omega) = \frac{1-\exp(-i\Omega t)}{\Omega}, \qquad \hbar\omega_{k,k+q} = E_k - E_{k+q}, \\ \Phi(\infty,\Omega) = \frac{1}{\Omega} + i\pi\delta(\Omega). \tag{24}$$

It should be noted, that the energy (22)–(24) of an electron of momentum k has a real part as well as imaginary part. Using the Eq. (21) at $\omega_1 = \omega_{k,k+q}$ and substituting it into the Eq. (23) gives for real part the expression

$$E_k^C = \sum_q V_q n_{k+q}\left(1 - \frac{1}{\varepsilon(q,\omega_{k,k+q})}\right) - \frac{1}{\pi}\sum_q V_q \int_{-\infty}^{\infty} d\omega \frac{n(\omega)+1}{\omega_{k,k+q}+\omega} \mathrm{Im}\left\{\frac{1}{\varepsilon^*(q,\omega)}\right\}. \tag{25}$$

Eqs. (18), (20), (23) and (25) are the main result of this section. Correlation contribution in the electron energy (25) is dependant on the dielectric function $\varepsilon(q,\omega)$ at $\omega = \omega_{k,k+q}$. Thus, energy E_k^C has to be calculated self consistently by an iteration method. As the first step by means of approximation

$$\varepsilon(q,\omega) = 1 + (\lambda_{F-T}q)^{-2} + \Delta\varepsilon(q,\omega), \\ \frac{1}{\varepsilon(q,\omega)} = \frac{1}{1+(\lambda_{F-T}q)^{-2}}\left(1 - \frac{\Delta\varepsilon(q,\omega)}{1+(\lambda_{F-T}q)^{-2}}\right), \\ \hbar\omega_{k,k+q} = e_k - e_{k+q} \tag{26}$$

we obtain for electron energy the equation

$$E_k = E_F\tilde{e}_k + \Delta E_k, \\ \Delta E_k = \sum_q \frac{V_q}{[1+(\lambda_{F-T}q)^{-2}]^2}\left[\Delta\varepsilon(q,\omega_{k,k+q})n_{k+q} - \frac{1}{\pi}\int_{-\infty}^{\infty} d\omega (n(\omega)+1)\mathrm{Im}\varepsilon(q,\omega)\right]. \tag{27}$$

Fermi–Thomas screening length λ_{F-T} exhibits a square root dependence on the density parameter r_s. The familiar expression for the screened exchange correction to the single electron energy is

$$E_F\tilde{e}_k = e_k - \sum_q \frac{V_q n_{k+q}}{[1+(\lambda_{F-T}q)^{-2}]}. \tag{28}$$

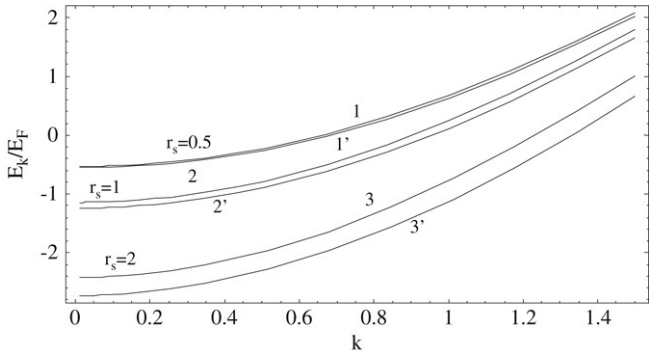


Fig. 1. Momentum k dependent electron energy at different values of the density parameter r_s. 1, 2, 3 – $\tilde{e}_k$ (29) and 1′, 2′, 3′ – E_k/E_F (27) at $r_s = 0.5, 1, 2$.

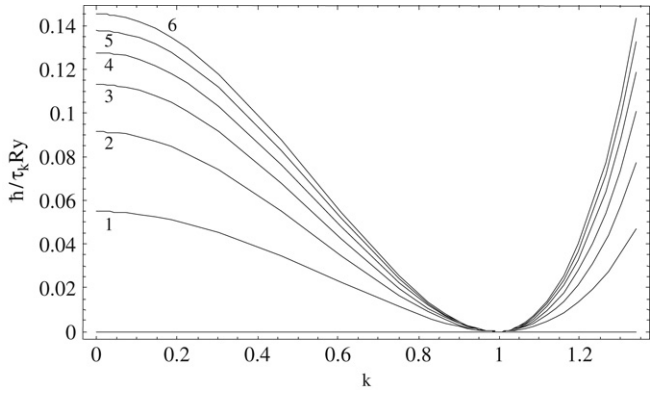


Fig. 2. The reciprocal lifetime versus momentum of an electron k computed by using Eqs. (32) and (33) at different values of the density parameter $r_s = 1, 2, 3, 4, 5, 6$ correspondingly.

The integration is quite straightforward and yields

$$\tilde{e}_k = k^2 - 0.5ar_s\left[1 + \frac{1-k^2+ar_s}{4k}\ln\left(\frac{ar_s+(k+1)^2}{ar_s+(k-1)^2}\right) - \sqrt{ar_s}\left(arctg\frac{1+k}{\sqrt{ar_s}} + arctg\frac{1-k}{\sqrt{ar_s}}\right)\right], \\ a = \left(\frac{4}{\pi\sqrt{3}}\right)^{4/3}. \tag{29}$$

The momentum k is expressed in units of the Fermi momentum k_F, $\tilde{e}_k$ is the electron energy measured in terms of Fermi energy $E_F = \hbar^2 k_F^2/2m$. The electron energies $\tilde{e}_k$ (29) and E_k/E_F (27) resulting from our model are presented in Fig. 1.

The energy of an electron E_k (27) is evaluated by making use of Lindhard's frequency and wave-number dependent dielectric function $\varepsilon(q,\omega)$. Numerical calculations have been carried out for different value of the density parameter r_s. At high density $r_s \ll 1$ the ΔE_k contribution (27) vanishing small and can be neglected, but it increases with decreasing density such that one obtains incorrect results if one ignores the contribution of ΔE_k (27) at $r_s \geq 1$.

The effective mass of the quasi-particles at the Fermi surface can be obtained by differentiating of $\tilde{e}_k$ with respect to momentum k evaluated at $k = 1$

$$\frac{m}{m^*} = 1 - 0.083r_s\left\{(1+0.332r_s)\ln\left[\frac{0.166r_s}{1+0.166r_s}\right] + 2\right\}. \tag{30}$$

Thus, in the limit of high density $r_s \to 0$ we have

$$\frac{m}{m^*} = 1 - 0.083r_s[\ln r_s + 0.203] \tag{31}$$

in agreement with Gell-Mann [10].

In addition to the energy, there is an attenuation of electron states. This damping is defined by the imaginary part of transition frequency of electrons and can be calculated by substituting $\Phi(\infty, \Omega)$ (24) into Eq. (23). The reciprocal lifetime is determined as

$$\frac{1}{\tau_k} = \frac{1}{\hbar}\sum_q \frac{V_q[n_{k+q} + n(\omega_{k,k+q})]}{[1 + (\lambda_{F-T}q)^{-2}]^2}\mathrm{Im}\varepsilon(q, \omega_{k,k+q}). \tag{32}$$

All integrals in the Eq. (32) can be evaluated explicitly and at $k \leq 1$ can be represented by the next expression.

$$\frac{\hbar}{\tau_k Ry} = \frac{2}{\pi}n_k[F(k) + F(-k)]$$

$$\begin{aligned} F(k) \;=\; & 0.25\left[\ln\left(\frac{ar_s + (k+1)^2}{ar_s(ar_s + 4k^2)}\right) + 0.5\right] \\ & + \frac{1 - k^2 + ar_s(3ar_s - 4k^2)}{8k(ar_s)^{3/2}}arctg\frac{1+k}{\sqrt{ar_s}} \\ & + (1+k)\frac{(1-k^2)^2 - ar_s(ar_s + 4k)}{8kar_s(ar_s + (k+1)^2)} \\ & + \frac{4k^2 - 3ar_s}{16k\sqrt{ar_s}}\left(arctg\frac{2k}{\sqrt{ar_s}}\right). \end{aligned} \tag{33}$$

Fig. 2 shows the dependence of the reciprocal lifetime on the momentum k at different values of parameter r_s, where $1/\tau_k$ is measured in the units of $Ry/\hbar$.

Dielectric function $\varepsilon(q, \omega)$ computed by Lindhard for degenerate electrons was used in calculation of $1/\tau_k$ (32) and (33). The numerical results obtained for lifetime τ_k as function of k and r_s are physically reasonable in view of experimental data [4].

References

[1] A.A. Klyukanov, A.V. Catanoi, Eur. Phys. J. B. 54 (2006) 275–281.
[2] A.A. Klyukanov, N.A. Loiko, I.V. Babushkin, V. Gurau, Proc. SPIE 4748 (2002) 301.
[3] A.A. Klyukanov, K.D. Sushkevich, M.V. Chukichev, A.Z. Awawdeh, V. Gurau, A.V. Catanoi, J. Optoel. & Adv. Mat., (JOAM) 8 (1) (2006) 123.
[4] V.P. Zhukov, O. Andreyev, D. Hoffman, M. Bauer, M. Aeschlimann, I.A. Nechaev, E.V. Chulkov, P.M. Echenique, Phys. Rev B. 70 (2004) 233106.
[5] G.F. Giuliani, G. Vignale, Quantum Theory of the Electron Liquid, Cambridge, 2005.
[6] I.V. Solovyev, Phys. Rev B. 73 (2006) 155117.
[7] P.M. Platsman, P.A. Wolf, Waves and Interactions in Solid State Plasmas, New York Ac., 1973.
[8] H. Kanazawa, S. Misawa, E. Fujita, Prog. Theor. Phys. 23 (3) (1960) 426.
[9] R. Zimmerman, K. Kilimann, W.D. Krafet, et al., Phys. Stat. Sol. B 90 (1) (1978) 175.
[10] M. Gell-Mann, Phys. Rev. 106 (1957) 359.