LETTER TO THE EDITOR

NOTE ON THE ELECTRON SCREENING FUNCTION AT LOW TEMPE-RATURES

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In evaluating the screening function in metals it is useful to approximate the actual one-electron energy by an analytically simple function of the wave number[1-5]. The approach which is widely used assumes that the energy is a quadratic function of the wave number. In an earlier paper this approximation was applied to the calculation of temperature effects in the dynamical screening function in degenerate semiconductors[6]. The aim of the present note is to improve this calculation by including the exchange and correlation contributions to the energy.

To determine the lowest-order temperature contribution to the screening function, it suffices to start from the $T = 0$ expression for energy. In the scheme of Bohm and Pines[7], the Hartree-Fock energy of an electron the wave number of which lies in the range $k_F - k_c < p < k_F + k_c$ is[8]

$$E = \frac{\hbar^2 p^2}{2m} - \frac{e^2}{2\pi\varepsilon}\left(k_F - 2k_c + \frac{k_F^3 - p^2}{p}\ln\frac{k_F + p}{k_c} + \frac{3}{2}p + \frac{k_c^2 - k_F^2}{2p}\right), \quad (1)$$

where ε is the dielectric constant of the media, while k_F and k_c are the Fermi and the cut-off wave number, respectively. With the help of (1) we arrive at the expression for the concentration

$$N = \frac{1}{3\pi^2} \left[p_\mu^3 + \frac{(\pi KT)^2}{6} \left(\frac{d^2}{dE^2} p^3 \right)_\mu \right] =$$

$$= \frac{p_\mu^3}{3\pi^2} \left\{ 1 + \frac{\pi^2}{8} \left(\frac{T}{T_F} \right)^2 \frac{1 - \gamma \left(\frac{7}{2} - \beta^2 - 3 \ln \frac{2}{\beta} \right)}{\left[1 - \gamma \left(1 - \frac{\beta^2}{4} - \ln \frac{2}{\beta} \right) \right]^3} \right\}. \tag{2}$$

Here we defined $\beta = k_c/k_F$, $T_F = \hbar^2 k_F^2/2mK$ and $\gamma = (4/9\pi^4)^{1/3} r_s$, with $r_s = (9\pi/4)^{1/3} me^2/\hbar^2 \, \varepsilon k_F$. After comparing (2) with $N = k_F^3/3\pi^2$, it follows

$$p_\mu = k_F \left\{ 1 - \frac{\pi^2}{24} \left(\frac{T}{T_F} \right)^2 \frac{1 - \gamma \left(\frac{7}{2} - \beta^2 - 3 \ln \frac{2}{\beta} \right)}{\left[1 - \gamma \left(1 - \frac{\beta^2}{4} - \ln \frac{2}{\beta} \right) \right]^3} \right\}. \tag{3}$$

In the limiting case, when electron exchange is neglected ($\gamma = 0$), relation (3) leads, of course, to the well-known expression for the chemical potential of an ideal Fermi gas $\mu = \mu(0) (1 - \pi^2 T^2/12T_F^2)$.

Table

r_s	β_1		β_2		β_3	
	Z_o	Z	Z_o	Z	Z_o	Z
0.1	1.008	0.948	1.007	0.956	1.006	0.968
0.2	1.015	0.918	1.013	0.933	1.012	0.953
0.3	1.021	0.896	1.019	0.919	1.016	0.943
0.4	1.026	0.880	1.024	0.908	1.021	0.937
0.5	1.031	0.867	1.028	0.901	1.026	0.933
0.6	1.036	0,856	1.033	0.897	1.030	0.930
0.7	1.041	0.848	1.037	0.894	1.034	0.930
0.8	1.046	0.841	1.041	0.893	1.038	0.930
0.9	1.051	0.835	1.045	0.893	1.042	0.931
1	1.055	0.831	1.049	0.894	1.046	0.934
1.5	1.076	0.823	1.068	0.913	1.064	0.954
2	1.096	0.830	1.084	0.947	1.081	0.986
2.5	1.114	0.848	1.100	0.992	1.097	1.026
3	1.131	0.875	1.115	1.047	1.112	1.073
3.5	1.148	0.909	1.129	1.110	1.128	1.126
4	1.164	0.950	1.143	1.181	1.143	1.185
4.5	1.179	0.998	1.156	1.259	1.157	1.250
5	1.194	1.054	1.169	1.344	1.171	1.320

Repeating the same procedure as in deriving expression (3), after a tedious but straightforward calculation, for the real part of the high-freguency long-wavelength electron polarizability we find

$$\text{Re } 4\pi\,\alpha\,(k,\,\omega) = -\frac{\omega_p^2}{\omega^2}\left\{1 + \frac{3k^2}{5\omega^2}v_F^2\left[1 - \gamma\left(1 + \frac{\beta^2}{4} - \frac{\beta^4}{8}\right) + \right.\right.$$

$$\left.\left. + \frac{5\pi^2}{12}\left(\frac{T}{T_F}\right)^2 Z\right]\right\}. \tag{4}$$

In (4), ω_p is the classical plasma frequency and Z is given by

$$Z = \frac{1}{\left[1 - \gamma\left(1 - \frac{\beta^2}{4} - \ln\frac{2}{\beta}\right)\right]^3}\left\{1 + \gamma\left(-\frac{9}{10} + \frac{4}{15}\beta^2 + \frac{17}{15}\ln\frac{2}{\beta}\right) - \right.$$

$$\left. - \frac{\gamma^2}{15}\left[\frac{3}{2} - \frac{\beta^2}{8} - \frac{\beta^4}{16} + \left(\frac{1}{2} - \frac{3\beta^2}{4} - 2\ln\frac{2}{\beta}\right)\ln\frac{2}{\beta}\right]\right\}. \tag{5}$$

Expression (5) has to be compared with the value calculated in the approximation that the electron energy is equal to $\hbar^2\,p^2/2m$[6]

$$Z_0 = 1 + \frac{\gamma}{10}\left(1 + \frac{\beta^2}{6} + \frac{4}{3}\ln\frac{2}{\beta}\right). \tag{6}$$

The numerical calculation is performed by choosing for β the following values: $\beta_1 = 0.353\sqrt{r_s}$[9], $\beta_2 = 0.470\sqrt{r_s}$[10] and β_3 determined by[11,12]

$$\left(1 + \frac{\beta_3}{2}\right)\ln\left(1 + \frac{2}{\beta_3}\right) = 1 + \frac{\beta_3^2}{2\gamma}. \tag{7}$$

As can be seen from the Table, the choice of β has no essential influence on the behaviour of both Z_0 and Z. This refers particularly to the region $r_s \le 1$, where we expect the non-RPA contributions to be small. In all the three cases Z_0 is a monotonously increasing function of β, while Z has a small drop in the region of high densities with a minimum in the vicinity of $r_s = 1$. In spite of that, the numerical values obtained in these two approaches differ for $r_s \le 5$ by no more than 20%.

It is somewhat surprising that even in the high-density limit, the deviation of Z from the RPA value $Z_{RPA} = 1$ is not negligible. This is the consequence of the logarithmic dependence of Z on β. Nevertheless, this deviation is not large, showing that the effect of electron exchange and correlation does not appreciably modify T^2 term in the screening function.

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