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Effect of screening on exchange effects for an inhomogeneous electron gas at finite temperatures

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Recently, Gupta and Rajagopal [Phys. Rev. A 21, 2064 (1980)] have calculated thermodynamic-exchange energy and potential in an "exchange-only" approximation and later calculated the correlation potential exactly within the random-phase approximation [Phys. Rev. A 22, 2792 (1980)]. In this paper we estimate the effect of screening in an approximate way. The formula obtained for the correlation potential is shown to be the product of two functions, one being that of density and the other being that of dimensionless temperature. The calculated values agree reasonably in the intermediate degeneracy region and are good at higher temperatures and densities. It is shown that the specific heat for the system can also be expressed in terms of the same parameters and the $(T/\ln T)$-type divergence disappears.

The density-functional approach of Hohenberg and Kohn has extensive applications for the zero-temperature ground-state properties of inhomogeneous electron gas systems.[1] The finite temperature generalization of the density-functional theory is due to Mermin[2] and it could have an interesting application in laser fusion theory. For this, one needs a form of exchange and correlation potential. Recently, Gupta and Rajagopal[3,4] have calculated the exchange and correlation potentials as well as the thermodynamic potentials for an inhomogeneous electron gas at finite temperatures. The same authors have discussed in detail the effect of screening on an impurity embedded in hot electron gas in the intermediate degeneracy region.[5] It is observed that in "exchange-only" approximation[3] one has $t = T/T_F$, where T is the temperature and T_F is the Fermi temperature, as the convenient variable, whereas to calculate the correlation potential one needs two out of the three variables, namely, t, T, and n, where n is the density.

The use of a Yukawa-type potential to study the correlation effects has a long and honorable history.[6] We have utilized a Yukawa-type potential[5] where the screening constant, which is related to the proper part of the polarization progagator, is evaluated for different temperatures and densities. To establish the notation, we write the thermodynamic potential $\Omega(n,T)$ as

$$\Omega(n,T) = \Omega_0(n,T) + \Omega_{\text{ex}}(n,T) + \Omega_r(n,T) \quad , \tag{1}$$

where $\Omega_0(n,T)$, $\Omega_{\text{ex}}(n,T)$, and $\Omega_r(n,T)$ are the contributions to the thermodynamic potential due to kinetic energy, exchange, and correlation, respectively. The exchange contribution is already evaluated in Ref. 3 where it is shown that $\Omega_{\text{ex}}(n,T)/\Omega_{\text{ex}}(n,0)$ is purely a function of t and hence is universal. The random-phase approximation (RPA) contribution to correlation potential is given by[7]

$$\Omega_r(n,T) = \frac{1}{2\beta(2\pi)^3} \int d^3q \sum_{\nu_n} \{\ln[1 - V(\vec{q})\Pi^{(0)}(\vec{q},\nu_n)] + V(\vec{q})\Pi^{(0)}(\vec{q},_n)\} \quad , \tag{2}$$

where we have used the notation of Ref. 7. This quantity has been evaluated numerically in Ref. 4. However, in this exact numerical evaluation the dependences of $\Omega_r(n,T)$ on density and temperature are not transparent. Here we show that if one makes the Yukawa-type screening approximation, one gets an almost closed-form solution for $\Omega_r(n,T)$. To this end we retain only the zero-frequency term in $\Pi^{(0)}(\vec{q},\nu_n)$ and take $q \to 0$ limit. Equivalence of this approximation to the Yukawa-type screening is discussed by Gupta and Rajagopal[5] in connection with the plasma screening effects. Using this approximation, the angular integration in Eq. (2) is easily carried out and we get the correlation part of thermodynamic potential per unit volume as

$$\Omega_r(n,T) = \frac{k_B T}{4\pi^2} \int_0^\infty \left[\ln\left(1 + \frac{a^2 k_F^2}{q^2} \right) - \frac{a^2 k_F^2}{q^2} \right] q^2\, dq \quad , \tag{3}$$

where

$$\begin{aligned} a^2 &= -4\pi e^2 \Pi^{(0)}(q \to 0, \nu = 0)/k_F^2 \\ &= \frac{4}{\pi a_0 k_F} \int_0^\infty \frac{dx}{e^{x^2/t - \alpha} + 1} \quad , \end{aligned} \tag{4}$$

and we have used the dimensionless variables $t = T/T_F$ and $\alpha = \mu/k_B T$. Here a_0 is the Bohr radius.

The integration in Eq. (2) is immediate and gives

$$\Omega_r(n,T) = -\frac{k_B T}{12\pi} a^3 k_F^3 \ . \tag{5}$$

By using n and t as independent variables, the above expression can be rewritten as

$$\frac{\Omega_r(n,t)}{N} = -\left[\left(\frac{3}{\pi}\right)^{1/6} \frac{e^2}{\sqrt{a_0}} (t I_1^{3/2})\right] n^{1/6} \ , \tag{6}$$

where

$$I_1 = \int_0^\infty \frac{dx}{e^{x^2/t-\alpha}+1} \ .$$

As has been shown in Ref. 3, α depends only upon t through a normalization condition

$$\tfrac{2}{3} t^{-3/2} = \int_0^\infty \frac{\sqrt{x}\, dx}{e^{x-\alpha}+1} \ . \tag{7}$$

Thus we see that $\Omega_r(n,t)/N$ is split up into the product of two distinct parts, one involving only t and the other involving only n.

Taking the functional derivative of $\Omega_r(n,t)/N$ with respect to the density n, we get the form for correlation potential $V_r(n,t)$ as[3]

$$V_r(n,t) = \left[\left(\frac{3}{\pi}\right)^{1/6} \frac{e^2}{\sqrt{a_0}} \left(t^2 I_1^{1/2} I_2 \frac{d\alpha}{dt}\right)\right] n^{1/6} \ , \tag{8}$$

where

$$I_2 = \int_0^\infty \frac{e^{x^2/t-\alpha}}{(e^{x^2/t-\alpha}+1)^2}\, dx \tag{9}$$

and

$$\frac{d\alpha}{dt} = -t^4/2I_\alpha \ ,$$

where

$$I_\alpha = \int_0^\infty \frac{y^2 e^{y^2/t-\alpha}}{(e^{y^2/t-\alpha}+1)^2}\, dy \ . \tag{10}$$

Since I_2 and I_α depend only on t, we see from Eq. (8) that $V_r(n,t)$, like $\Omega_r(n,t)/N$, splits into the product of two distinct functions of t and n, respectively.

It is easily verified that the equations for $\Omega_r(n,t)/N$ and $V_r(n,t)$ reduce to the correct high-temperature limit.[4,8] For the low-temperature case, our results do not reproduce the correct behavior. This is expected because we are completely neglecting the dynamical effects by retaining only one term in the frequency sum.

We have made the detailed comparison with the exact numerical calculations in RPA of Gupta and Rajagopal[3,4] and our results are shown in Table I. As expected, the correlation potential is overestimated in the present approximation. It is seen that for large t and high n the agreement is very good. The low t values are as much as 100% off from the correct values. However, at low temperatures, exchange predominates over correlations and hence the effect of correlation is expected to be small. This is clearly seen from the total value of the exchange and correlation potentials denoted by the suffix xc [e.g., $\Omega_{\text{xc}}(n,t) = \Omega_{\text{ex}}(t) + \Omega_r(n,t)$] and given in Table I. The contribution of the exchange part to $\Omega_{\text{xc}}(n,t)$ and $V_{\text{xc}}(n,t)$ depends only on t and is taken directly from Ref. 3. Figures 1 and 2 show the behavior of $\Omega_{xc}(n,t)/N$ and $V_{xc}(n,t)$ for different values of T. It is seen that in the intermediate degeneracy region the total value of the exchange-correlation part does not differ from its exact counterpart by more than about 5 to 10%.

We employ the same approximation to calculate the specific heat of the inhomogeneous system. As shown by Garrison,[9] the effect of screening on specific heat is rather drastic. We therefore decided to see the behavior of specific heat at different temperatures. To evaluate the specific heat we use the expression, due to Bardeen, as

$$\frac{C_{\text{xc}}}{C_0} = \frac{\hbar^2 k_F}{m(\partial\epsilon_k/\partial k)_{k_F}} \ , \tag{11}$$

where C_{xc} is a specific heat of interacting electron gas and C_0 is a corresponding specific heat for a noninteracting system.

Here ϵ_k is a single-particle excitation spectrum. If $V_s(\vec{k})$ is the screened Coulomb potential, given by

$$V_s(\vec{k}) = \frac{4\pi e^2}{k^2 - 4\pi e^2 \pi^{(0)}(\vec{k},0)} \ ,$$

we write[10]

$$\epsilon_k = \frac{\hbar^2 k^2}{2m} - \sum_{\vec{k}'} V_s(|\vec{k}-\vec{k}'|) f(\epsilon_{k'}) \ , \tag{12}$$

where $f(\epsilon_k)$ is a Fermi function. By using Eq. (3), Eq. (11) can be transformed into the "t" variable as

$$\frac{C_0}{C_{\text{xc}}} = 1 - \frac{t}{4\pi a_0 k_F}\left[2\int_0^\infty \frac{dy}{e^{y-\alpha}+1}\left(\frac{1+\sqrt{ty}}{(1+\sqrt{ty})^2+a^2} - \frac{1-\sqrt{ty}}{(1-\sqrt{ty})^2+a^2}\right) - \int_0^\infty \frac{dy}{e^{y-\alpha}+1} \ln\left|\frac{(1+\sqrt{ty})^2+a^2}{(1-\sqrt{ty})^2+a^2}\right|\right] \ . \tag{13}$$

As shown by Garrison *et al.*,[9] the Yukawa-type screening approximation that is used here gives reasonably good values of C_0/C_{xc} at $T=0$. We therefore expect that, for specific-heat calculation, Eq. (13) may not be a bad approximation over the entire temperature range.

TABLE I. Values of the exchange-correlation potential $V_{xc}(n,t)$ and the thermodynamic potential $\Omega_{xc}(n,t)$ as a function of t for different electron densities. The correlation contributions are also tabulated. The starred values are from Ref. 4. (All energy units in rydberg.) Subsections (a), (b), and (c) denote different values of n.

t	$-\Omega_r/N$	$-\Omega_r^*/N$	$-\Omega_x^*/N$	$-\Omega_{xc}/N$	$-\Omega_{xc}^*/N$	$-V_r$	$-V_r^*$	$-V_x^*$	$-V_{xc}$	$-V_{xc}^*$
(a) $n=10^{26}$ cm^{-3} ($T_F=9.1\times10^6$ K)										
0.1	0.308	0.350	3.479	3.787	3.829	0.160	0.281	4.794	4.954	5.075
0.3	0.807	0.704	2.812	3.619	3.516	0.565	0.532	4.475	5.040	5.007
0.6	1.134	0.976	1.988	3.122	2.964	1.122	0.959	3.488	4.610	4.447
1.0	1.201	1.054	1.386	2.587	2.440	1.431	1.229	2.574	4.005	3.803
1.5	1.130	1.022	0.987	2.117	2.009	1.494	1.308	1.843	3.227	3.151
2.0	1.050	0.963	0.762	1.812	1.725	1.441	1.291	1.480	2.921	2.771
2.5	0.976	0.905	0.620	1.596	1.525	1.368	1.246	1.214	2.582	2.460
3.0	0.911	0.853	0.541	1.452	1.394	1.300	1.194	1.084	2.384	2.278
3.5	0.857	0.807	0.464	1.321	1.271	1.233	1.144	0.924	2.157	2.068
4.0	0.808	0.767	0.403	1.211	1.170	1.175	1.097	0.806	1.981	1.903
4.5	0.769	0.732	0.358	1.127	1.090	1.122	1.054	0.717	1.839	1.771
5.0	0.735	0.701	0.323	1.058	1.024	1.076	1.014	0.645	1.721	1.659
10.0	0.531	0.530	0.161	0.692	0.691	0.790	0.792	0.323	1.113	1.115
(b) $n=10^{24}$ cm^{-3} ($T_F=4.2\times10^5$ K)										
0.1	0.143	0.177	0.750	0.893	0.927	0.074	0.169	1.033	1.107	1.202
0.3	0.374	0.288	0.606	0.980	0.894	0.262	0.236	0.964	1.226	1.200
0.6	0.527	0.390	0.428	0.955	0.818	0.521	0.382	0.751	1.272	1.133
1.0	0.557	0.429	0.299	0.856	0.728	0.664	0.488	0.555	1.219	1.043
1.5	0.524	0.426	0.213	0.737	0.639	0.693	0.531	0.397	1.090	0.928
2.0	0.487	0.408	0.164	0.651	0.572	0.669	0.534	0.319	0.988	0.853
2.5	0.453	0.388	0.134	0.587	0.522	0.635	0.523	0.262	0.897	0.785
3.0	0.423	0.369	0.117	0.540	0.486	0.603	0.507	0.234	0.837	0.741
3.5	0.398	0.352	0.100	0.498	0.452	0.572	0.490	0.199	0.771	0.689
4.0	0.375	0.337	0.087	0.462	0.424	0.545	0.473	0.174	0.719	0.647
4.5	0.357	0.323	0.077	0.434	0.400	0.521	0.461	0.154	0.675	0.615
5.0	0.341	0.311	0.070	0.411	0.381	0.499	0.443	0.139	0.638	0.582
10.0	0.247	0.240	0.035	0.282	0.275	0.367	0.365	0.070	0.437	0.435
(c) $n=10^{22}$ cm^{-3} ($T_F=2.0\times10^4$ K)										
0.1	0.066	0.086	0.162	0.228	0.248	0.034	0.093	0.223	0.257	0.316
0.3	0.174	0.111	0.131	0.305	0.242	0.122	0.105	0.208	0.330	0.313
0.6	0.244	0.141	0.092	0.336	0.233	0.242	0.141	0.162	0.404	0.303
1.0	0.259	0.158	0.064	0.323	0.222	0.308	0.175	0.120	0.428	0.295
1.5	0.243	0.162	0.046	0.289	0.208	0.322	0.194	0.086	0.408	0.280
2.0	0.226	0.159	0.0305	0.261	0.194	0.310	0.1996	0.069	0.379	0.269
2.5	0.210	0.155	0.029	0.239	0.184	0.295	0.2001	0.056	0.351	0.256
3.0	0.196	0.150	0.025	0.221	0.175	0.280	0.198	0.050	0.330	0.248
3.5	0.185	0.144	0.022	0.207	0.166	0.266	0.194	0.043	0.309	0.237
4.0	0.174	0.140	0.019	0.193	0.159	0.253	0.190	0.037	0.290	0.227
4.5	0.166	0.135	0.017	0.183	0.152	0.242	0.186	0.033	0.275	0.219
5.0	0.158	0.131	0.015	0.173	0.146	0.232	0.181	0.030	0.262	0.211
10.0	0.114	0.108	0.008	0.122	0.116	0.170	0.161	0.015	0.185	0.176

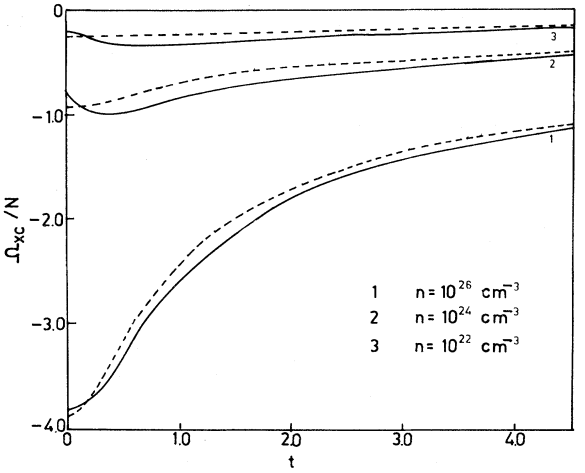

FIG. 1. Exchange-correlation thermodynamic potential $\Omega_{xc}(n,T)$ as a function of t for different electron densities. The dashed curves are drawn using values from Ref. 4.

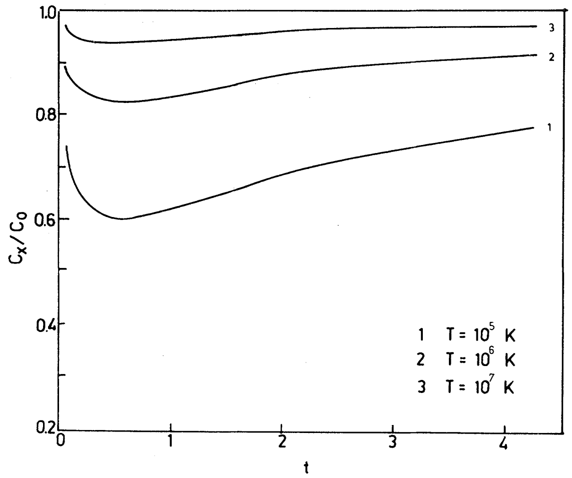

FIG. 3. Variation of C_x/C_0 with t in exchange-only approximation for different temperatures.

For small t, by using the procedure given in Ref. 11,

$$\frac{C_0}{C_{xc}} \simeq 1 + \frac{1}{4\pi a_0 k_F}\left[(2+a^2)\ln\frac{4+a^2}{a^2} - 4\right] \tag{14}$$

or

$$\frac{C_0}{C_{xc}} \simeq 1 + \frac{e^2}{4\pi}\left[\frac{m}{2\hbar^2 k_B T}\right]^{1/2} \times (c_1 t^{1/2} - t^{1/2}\ln t + C_2 t - C_3 t\ln t) \;, \tag{14a}$$

where

$$C_1 = 2\ln\frac{4}{A} - 4, \quad C_2 = A\ln\frac{4}{A} + \frac{A}{2}, \quad C_3 = \frac{A}{2} \;,$$

and

$$A = \frac{4e^2}{\pi\hbar}\left[\frac{m}{2k_B T}\right]^{1/2} \;.$$

The ratio C_0/C_x as calculated by Bardeen is quoted by Wohlforth[12] and is supposed to be valid for low temperatures in exchange-only approximation. It is

$$\frac{C_0}{C_x} \simeq 1 + \frac{4\pi}{a_0 k_F}\ln\frac{2e^2 k_F}{\pi k_B T} \;. \tag{15}$$

This result gives a singularity of the type $T/(\ln T)$ in

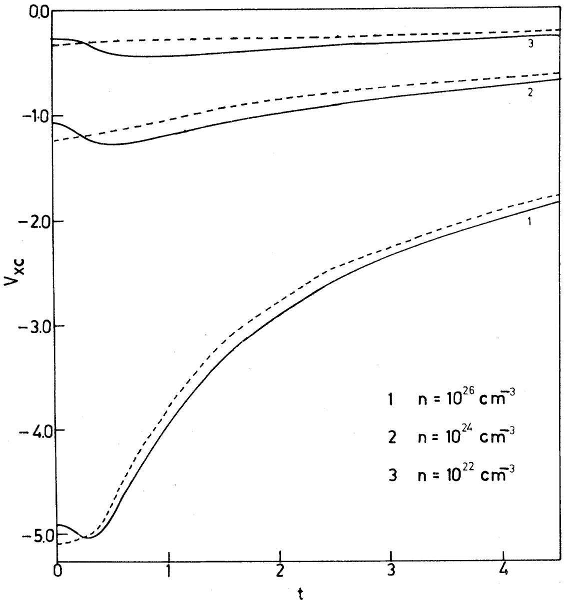

FIG. 2. Exchange-correlation potential $V_{xc}(n,T)$ as a function of t for different electron densities. The dashed curves are drawn using values from Ref. 4.

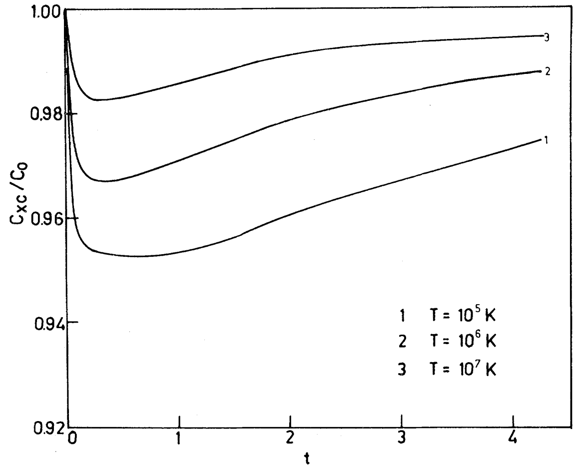

FIG. 4. Variation of C_{xc}/C_0 with t in exchange-screening approximation for different temperatures.

specific heat at low temperature. This should be compared with our small t result. It is easily seen from Eq. (14a) that, upon substitution of the value of A, $\ln T$ divergence disappears. Figure 3 shows the variation of C_x/C_0 in exchange-only approximation with t, i.e., using formula (13) with $a^2=0$. Figure 4 indicates the variation of C_{xc}/C_0 in "exchange-screening" approximation with t. For large temperatures or small densities the ratio, as expected, approaches unity in both cases. However, the effect of screening is substantial, as can be seen from Fig. 4.

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