von Weizsäcker coefficient for high-temperature electron plasmas

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The coefficient of the von Weizsäcker term in the Thomas–Fermi–von Weizsäcker energy functional is determined within a perturbation framework for high-temperature plasmas. A notable deviation in comparison to the corresponding zero-temperature result is found.

There is a renewed interest for using classical density-functional theory (CDFT) in problems that have an intrinsic many-body nature. An interesting example is the problem of atoms in plasmas.[1-3] CDFT is conceptually simple and does not require a preliminary calculation of the individual electronic wave functions.[4] On the other hand, the applied direct approximations to the kinetic energy, or Helmholtz's free energy at nonzero temperature, need theoretical justifications in CDFT.

The standard Thomas–Fermi–von Weizsäcker (TFW) approximation for the kinetic energy in question contains a parameter λ. The determination of this λ parameter is based on different physical requirements.[5-8]

In the present Brief Report we determine the λ parameter by using a perturbative description for the energy change caused by an effective screened external potential $V(r)$ in high-temperature electronic plasmas.

According to the result of Meyer, Wang, and Young[9] the second-order energy change $[\Delta E^{(2)}]$ is as follows:

$$\Delta E^{(2)}=\frac{1}{2}\frac{1}{(2\pi)^3}\int_0^\infty(4\pi q^2 dq)|V(q)|^2\Pi(q) , \tag{1}$$

in which $V(q)$ is the Fourier transform of $V(r)$ and $\Pi(q)$ is the screened response function (or free electron polarization propagator) of the noninteracting system (see also Refs. 10 and 11). The exact random-phase approximation (RPA) response function is

$$\Pi^{\mathrm{RPA}}(q,T)=\frac{n_0}{kT}\exp\left[-\frac{q^2}{8kT}\right]\sum_{n=0}^{\infty}\frac{1}{2n+1}\frac{1}{n!}\left[\frac{q^2}{8kT}\right]^n \tag{2}$$

in the examined high-temperature limit, where n_0 is the density of the host system, T is the temperature, and k is the Boltzmann constant. To deduce Eq. (2) we have used the so-called real-space RPA response function[12]

$$\Pi^{\mathrm{RPA}}(R,T)=\frac{n_0}{\pi}\frac{1}{R}\exp(-2kTR^2) , \tag{3}$$

where $R=|\mathbf{r}-\mathbf{r}'|$, and we have performed a Fourier transformation for it.

In the TFW λ approximation the response function is given by[13]

$$\Pi^{\lambda}(q,T)=\frac{n_0}{kT}\frac{1}{1+\lambda(q^2/4kT)} \tag{4}$$

for high temperatures. It is easy to show that (i) $\Pi^{\lambda=1}=\Pi^{\mathrm{RPA}}$ in the short-wavelength ($q\to\infty$) limit, and (ii) $\Pi^{\lambda}=\Pi^{\mathrm{RPA}}$ at $q=0$ independently of λ.

If the approximate method [see Eq. (4)] is to give the exact energy change [see Eqs. (1) and (2)] in the weak-coupling limit, then the natural requirement is the following:

$$\int_0^\infty dq\, q^2[\Pi^{\lambda}(q,T)-\Pi^{\mathrm{RPA}}(q,T)]|V(q)|^2=0 . \tag{5}$$

Here we specify the effective potential $V(r)$ as a simple Yukawa type, given by

$$V(r)=\frac{1}{r}e^{-\alpha r}$$

and solve Eq. (5) for the optimal λ value. Because we are interested in the asymptotic behavior (see next paragraph) the noninteracting picture of the system and the use of a Yukawa potential are fully satisfactory. The same result holds in the Hartree self-consistent-field description.

The integration can be performed without difficulty due to the fast convergence of the series in Eq. (2). The results that we have obtained for the λ parameter are plotted in Fig. 1 as a function of the reduced variable $x=\alpha^2/4kT$. For very high temperatures ($x\to 0$) the op-

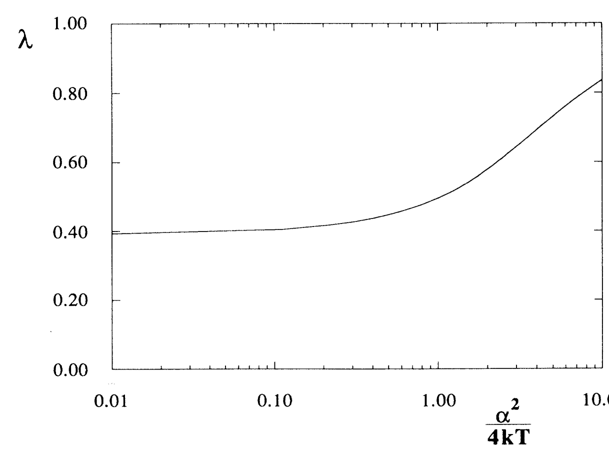

FIG. 1. The values of the von Weizsäcker coefficient λ as a function of the reduced variable $x=\alpha^2/4kT$. For $x\to\infty$ λ tends to unity. See the text for further details.

timal value, predicted by the applied constraint [see Eq. (5)], is about $\lambda = 0.393$. This Coulombic limit value is roughly two times bigger than the corresponding zero-temperature result ($\lambda = 0.205$) of Meyer, Wang, and Young.[9] [The forms of $\Pi(q)$ are different at $T=0$; see Ref. 9.] It is worth mentioning that a required equivalence of Eqs. (2) and (4) for small-q values gives the $\lambda = \frac{1}{3}$ value, as it is well known.[6,14] In conclusion, in the high-temperature limit the *mentioned* restrictions predict nearly equivalent λ values.

We have to stress, however, that the outlined theoretical framework is a perturbative method, for the second-order energy change $\Delta E^{(2)}$. In the limiting case [T is very high, therefore $\alpha \sim (n_0/kT)^{1/2}$] the leading first-order energy change ($\Delta E^{(1)}$) is independent of the λ value, namely $\Delta E^{(1)} \sim n_0/[\Pi(q=0)]$, and *only* $\lambda = 1$ is compatible with the nuclear-cusp condition.[6,13]

We finish our consideration by writing an integral-representation form for $\Pi^{\mathrm{RPA}}(q,T)$. Using the notation $s^2 = q^2/8kT$ and observing that the series in Eq. (2) refers to the ${}_1F_1(\frac{1}{2},\frac{3}{2},s^2)$ confluent hypergeometric function, we arrive at the desired result

$$\Pi^{\mathrm{RPA}}(q,T) = \frac{n_0}{kT} e^{-s^2} \frac{1}{s} \int_0^s du\, e^{u^2} . \tag{6}$$

The expression in Eq. (6) is the so-called Fried-Conte function.[15] For practical applications powerful two-sided Padé approximants of the above function are available.[16] It turns out that the first nontrivial two-sided Padé approximant of Németh, Ag, and Páris[16] (determined on mathematical grounds) is equivalent to our physical result given by Eq. (4) for $\lambda = 1$.

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