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COMMENT

## The kinetic energy density functional for fast-varying densities

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**Abstract.** We argue, by giving an explicit example, that the class of trial functions used by Lee and Chuu in deriving the kinetic energy density functional for systems with fast-varying densities is unrealistic for many systems of current interest. Therefore, in contrast to their conclusion, the applicability of their results is quite limited.

Recently Lee and Chuu (1988) used a variational method to derive the kinetic energy density functional of an inhomogeneous fermion gas with a correction term<sup>†</sup>

$$\Delta t_s(n(\mathbf{r})) = (\hbar^2/8m)|\nabla n(\mathbf{r})/n(\mathbf{r})|^2 \quad (1)$$

which they claimed to be valid even when the density  $n(\mathbf{r})$  varies rapidly. However, the validity of their conclusions is questionable for many systems of current interest, because the class of trial wavefunctions they used is unrealistic.

It is the purpose of this Comment to explain why the class of trial wavefunctions used by Lee and Chuu is unrealistic for many systems and to give an explicit example to support our argument.

The class of trial single-particle wavefunctions used by Lee and Chuu is of the following form, with the density varying rapidly in the  $z$  direction

$$\psi_{k_x, k_y}(x, y, z) = (1/\sqrt{A}) \exp(ik_x x + ik_y y) \varphi_0(z). \quad (2)$$

They argued that from the variational point of view a single  $\varphi_0(z)$  for all particles would lower the energy. However, we think this argument is in general wrong. For example, we may consider a semi-infinite metal with a surface at  $z = 0$  ( $z > 0$  is the vacuum). The single-particle wavefunction deep inside the bulk is not affected by the presence of the surface and can be taken as a plane wave

$$\psi_{\text{bulk}}(x, y, z) = (1/\sqrt{V}) \exp(ik_x x + ik_y y) \sin(k_z z - \gamma) \quad (3)$$

where we have taken the  $x$ - and  $y$ -component wavefunctions to be the same as in (2). The phase angle  $\gamma$  represents a phase shift due to the presence of the surface. The

<sup>†</sup> It is also worthwhile to note that (1) is the only correction term they obtained; i.e., there is no other correction term to any order.

wavefunctions (2) and (3) must represent the same state with (3) as the asymptotic form of (2).

In the ground state electrons fill up the levels of  $k_z$  from 0 to  $k_F$ ; it is therefore apparent that a single  $\varphi_0(z)$  will not be sufficient to accommodate all electrons in the metal. Therefore Lee and Chuu's argument is wrong, at least for this particular system.

To give a precise derivation of the electron density of the above system, we quote the work of Lang and Kohn (1970). They used the Kohn–Sham self-consistent differential equation to calculate the surface charge density. We write down the relevant equations in the following. The eigenfunction is written in the form

$$\varphi_{k_x, k_y, k}(x, y, z) = \exp(ik_x x + ik_y y) \varphi_k(z) \quad (4a)$$

where, for  $z \rightarrow -\infty$ ,

$$\varphi_k(z) = \sin(kz - \gamma(k)). \quad (4b)$$

The self-consistent equation to be solved is

$$\left(-\frac{1}{2} \frac{d^2}{dz^2} + v_{\text{eff}}[n; z]\right) \varphi_k(z) = \frac{1}{2}(k^2 - k_F^2) \varphi_k(z) \quad (5)$$

where atomic units have been used and  $v_{\text{eff}}$  is the effective potential whose explicit expression will not be given here. The electron density is given by

$$n(z) = \frac{1}{\pi^2} \int_0^{k_F} (k_F^2 - k^2) (\varphi_k(z))^2 dk. \quad (6)$$

It is easily seen from (5) that it is impossible to obtain a  $k$ -independent solution  $\varphi_k(z)$ . Therefore the density obtained by Lee and Chuu

$$n(r) = (N(\Delta z)/A) |\varphi_0(z)|^2 \quad (7)$$

is not compatible with the calculated ground-state electron density (6). It is therefore clear that Lee and Chuu's results cannot be applied to a metal surface.

We can also think of other systems, such as multi-electron atoms, molecules, and films that are not too thin etc, for which Lee and Chuu's results are not applicable because in these systems a single  $z$ - (or radial) component wavefunction is not sufficient to accommodate all electrons. The only systems we can think of for which Lee and Chuu's results may be applicable are two-electron atoms (or ions) and, perhaps, ultra-thin films, in which a single  $z$ - (or radial) component wavefunction may be sufficient to accommodate all electrons. But for the latter systems the problem is complicated by the interface interactions and no clear-cut conclusion can be drawn.

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## References

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