Self-consistent kinetic energy in the electron fluid

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(Received 22 November 1982)

A self-consistent expression for the kinetic energy of a fermion Jastrow trial function is derived. Calculations for the electron fluid show only a small shift from earlier results using the Clark-Westhaus kinetic energy with the convolution approximation.

I. INTRODUCTION

The Feenberg-Jastrow variational theory has been applied extensively to the theory of highly correlated quantum fluids with much success. These fluids include both the electron fluid, with its *long-range* Coulomb interaction,[1] and systems with *short-range* interactions such as the helium liquids[2] and nuclear matter. When applying integral-equation methods to evaluate the energy in these systems [most notably the hypernetted-chain approximation (HNC) and its generalizations], it is necessary to choose between several formally equivalent expressions for the kinetic energy, the most common of which are the Jackson-Feenberg (JF), Clark-Westhaus (CW), and Pandharipande-Bethe expressions.[3] Each expression has advantages and disadvantages. It was shown in Ref. 1, for example, that the CW kinetic energy used with the effective-correlation HNC approximation gives very good results for the electron fluid over a wide density range. On the other hand, the JF kinetic energy is generally preferred for short-ranged systems because the three-body term in the kinetic energy in those systems is small and the resultant Euler-Lagrange equations are well behaved.

In Ref. 2 it was shown that the differences between these evaluations of the kinetic energy are due to inconsistent approximations for the two- and three-body terms in these forms. It was pointed out that the fermion generalization of the Born-Green-Yvon equations (FBGY) removes this inconsistency. The natural approximations within the FBGY method are not, however, stable under Euler-Lagrange analysis, in contrast to the HNC-based approximations.

Another possible resolution of the kinetic energy difficulties is to make use of the fact that, while three-body functions appear in the kinetic energy, the HNC equations depend only on the two-body distribution function and other related two-body functions. Thus a suitably chosen HNC approximation for the three-body functions will render all of the kinetic energies equivalent.[2]

Since the three-body term in the JF kinetic energy is ignorable in *short-ranged systems,* such a self-consistent approximation scheme is unnecessary; it would merely bring the other evaluations into agreement with the JF value. Such is not the case, however, in the electron fluid where the three-body terms are important in each of the alternative expressions. Our purpose in this Brief Report is to develop an HNC-consistent expression for the kinetic energy and to investigate its effect in the electron fluid.

II. SELF-CONSISTENT KINETIC ENERGY

The Jastrow trial wave function for an N-body fermion system has the form

$$\psi(\vec{r}_1,\ldots,\vec{r}_n)=\phi(\vec{r}_1,\ldots,\vec{r}_n)\prod_{i<j}^{N}e^{u(r_{ij})/2}\ , \quad (1)$$

where ϕ is the ground-state Slater determinant of the noninteracting system and $u(r)$ is chosen to minimize the expectation value of the Hamiltonian. The CW expression for the kinetic energy is

$$\frac{\langle T\rangle}{N}=T_\phi+T_2+T_3=\frac{3}{5}\frac{\hbar^2}{2m}k_F^2+\rho\int d^3r\,g(r)\frac{\hbar^2}{8m}[\vec{\nabla}u(r)]^2$$
$$+\rho^2\int d^3r_{12}\int d^3r_{23}g_3(\vec{r}_{12},\vec{r}_{23})\frac{\hbar^2}{8m}\vec{\nabla}_2u(r_{12})\cdot\vec{\nabla}_2u(r_{23})\ , \quad (2)$$

where $g(r_{12})$ is the two-body (or radial) distribution function

$$g(r_{12})=\frac{N(N-1)}{\rho^2}\frac{\int d^3r_3\cdots d^3r_N|\psi|^2}{\int d^3r_1\cdots d^3r_N|\psi|^2} \quad (3)$$

and g_3 is the similarly defined three-body distribution function.

To eliminate the three-body term in Eq. (2) in favor of two-body functions, we define an operator $\vec{\partial}$ which has the same effect as the ordinary gradient $\vec{\nabla}$ except that it operates only on the $\vec{r}$ dependence

through the Jastrow pseudopotential u. Then the equation $\vec{\delta} g$ looks like the ordinary BGY equation

$$\vec{\delta}_1 g(r_{12}) = g(r_{12}) \vec{\nabla}_1 u(r_{12}) + \rho^2 \int g_3(\vec{r}_{12}, \vec{r}_{23}) \vec{\nabla}_1 u(\vec{r}_{13}) d^3 r_3 \ . \quad (4)$$

Using Eq. (2) we obtain

$$T_2 + T_3 = \rho \int d^3 r_{12} \frac{\hbar^2}{8m} \vec{\nabla}_1 u(r_{12}) \cdot \vec{\delta}_1 g(r_{12}) \quad (5)$$

which is a natural generalization of the boson Jackson-Feenberg kinetic energy.[4]

We shall refer to an approximation as *self-consistent* if it uses the same approximate functional relationship between g and u to generate the approximation for $\vec{\delta} g$.

III. APPROXIMATION

A simple but useful application of this result is obtained by using the effective-correlation (i.e., Lado) HNC approximation for $g(r)$ (Ref. 1):

$$g(r) = \exp[u(r) + w(r) + N(r)] \ , \quad (6)$$

where $w(r)$ is chosen to reproduce the noninteracting fermion radial distribution function when $u(r) = 0$, and $N(r)$ is the nodal function defined by the equation

$$N(r) = \rho \int X(\vec{r} - \vec{r}')[g(\vec{r}') - 1] d^3 r' \ , \quad (7)$$

where $X(r)$ is the direct correlation (or non-nodal) function satisfying the nodal equation

$$g(r) - 1 = X(r) + N(r) \ . \quad (8)$$

Then if we define the auxiliary functions $\eta(\vec{r}), \xi(\vec{r})$ by

$$\vec{\nabla} \eta(r) = \vec{\delta} N(r), \quad \vec{\nabla} \xi(r) = \vec{\delta} X(r), \quad (9)$$

the equations for $\vec{\delta} g$ generated by Eqs. (6)–(8) are

$$\vec{\delta} g(r) = \vec{\nabla} g(r) + g(r) \vec{\nabla} \times [\eta(r) - w(r) - N(r)] \ , \quad (10)$$

where

$$\vec{\nabla} \eta(r) = \rho \int \vec{\nabla} \xi(\vec{r} - \vec{r}')[g(r') - 1] d^3 r' \quad (11)$$

and

$$\vec{\delta} g(r) = \vec{\nabla} \xi(r) + \vec{\nabla} \eta(r) \ . \quad (12)$$

Note that Eq. (10) may be used to express the kinetic energy in the following form:

$$T_2 + T_3 = \rho \int d^3 r \frac{\hbar^2}{8m} \vec{\nabla} u(r) \cdot \vec{\nabla} g(r) + \rho \int d^3 r \frac{\hbar^2}{8m} g(r) \vec{\nabla} u(r) \cdot \vec{\nabla} [\eta(r) - w(r) - N(r)] \ . \quad (13)$$

The second term is the fermion correction to the boson JF form; it vanishes in the boson limit, where $w = 0$ and $\eta(r) = N(r)$.

IV. ELECTRON FLUID

Special care must be taken with the large-r properties of any approximation used with the electron fluid. For this reason the convolution approximation (CA) was used in the CW kinetic energy in Ref. 1.

The resulting Euler-Lagrange equation,

$$\frac{\delta}{\delta u(r)} \langle H \rangle = 0 \ , \quad (14)$$

is well-behaved, and the solutions satisfy the perfect screening long-wavelength limit. Adding low-order HNC-type corrections to T_3 made only small shifts in the energy (see below), though incorporating these corrections in the energy before deriving the Euler-Lagrange equation introduces improper long-wavelength behavior. To facilitate comparison between the CA results of Ref. 1 and our self-consistent (SC) approximation using Eq. (13), we define the energy shift

$$\Delta T \equiv T_3^{\mathrm{SC}} - T_3^{\mathrm{CA}} = \frac{\hbar^2}{8m} \frac{1}{(2\pi)^3 \rho} \int d^3 k \int dp \int_{|p-k|}^{p+k} dq \ C_{pq}^k [S(k) - 1] u(p) S(p) [y(q) - u(q) S(q)] \ , \quad (15)$$

where $S(k) - 1$ and $u(k)$ are the dimensionless Fourier transforms of $g(r) - 1$ and $u(r)$, respectively, C_{pq}^k is a phase-space factor defined in Ref. 1, and $y(k)$ is the dimensionless Fourier transform of $\eta(r) + u(r)$ satisfying Eqs. (10)–(12) which can be rewritten as a linear integral equation:

$$k^2 y(k) = k^2 u(k) S(k) + \frac{[S(k) - 1]}{8\pi^2 \rho} \int_0^\infty dp \int_{|p-k|}^{p+k} dq \frac{pq}{k} (k^2 + p^2 - q^2)[S(p) - 1] y(q) \ . \quad (16)$$

TABLE I. The correlation energy per particle of the electron fluid at several densities (measured by r_s) and spin degeneracies ν, in millirydberg units. E^{CA}: Results of Ref. 1 using the convolution approximation in the CW energy. ΔT^{SC}: The energy difference between the self-consistent approximation and the convolution approximation. ΔT^{LO}: Lowest-order HNC corrections to the convolution approximation (Ref. 1).

	$\nu=1$			$\nu=2$			$\nu=4$		
r_s	E^{CA}	ΔT^{SC}	ΔT^{LO}	E^{CA}	ΔT^{SC}	ΔT^{LO}	E^{CA}	ΔT^{SC}	ΔT^{LO}
1	−53.9	−0.75	−0.31	−113	−0.72	−0.62	−182	−0.55	−0.51
2	−41.0	−0.62	−0.28	−85	−0.69	−0.67	−132	−0.63	−0.63
4	−30.0	−0.48	−0.24	−60.4	−0.60	−0.65	−90.4	−0.62	−0.68
6	−24.4	−0.40	−0.20	−48.1	−0.51	−0.59	−70.3	−0.55	−0.64
8	−20.9	−0.34	−0.17	−40.4	−0.43	−0.52	−58.1	−0.48	−0.57
10	−18.4	−0.29	−0.14	−35.0	−0.37	−0.46	−49.8	−0.41	−0.51
14	−15.1	−0.23	−0.09	−27.9	−0.28	−0.35	−39.0	−0.31	−0.39
20	−12.1	−0.17	−0.04	−21.6	−0.20	−0.23	−29.7	−0.22	−0.26
30	−9.18	−0.11	0.02	−15.9	−0.12	−0.11	−21.6	−0.13	−0.13
40	−7.50	−0.08	0.05	−12.7	−0.08	−0.04	−17.0	−0.09	−0.05
50	−6.38	−0.06	0.07	−10.6	−0.05	0.00	−14.1	−0.06	−0.01

	$\nu=8$			$\nu=\infty$		
r_s	E^{CA}	ΔT^{SC}	ΔT^{LO}	E^{CA}	ΔT^{SC}	ΔT^{LO}
1	−261	−0.52	−0.47	−775	−0.59	−0.45
2	−181	−0.64	−0.62	−449	−0.73	−0.61
4	−119	−0.66	−0.69	−257	−0.72	−0.68
6	−90.7	−0.59	−0.65	−184	−0.64	−0.64
8	−74.0	−0.51	−0.58	−144	−0.55	−0.57
10	−62.8	−0.44	−0.52	−119	−0.47	−0.50
14	−48.6	−0.34	−0.39	−89.3	−0.36	−0.38
20	−36.6	−0.23	−0.26	−65.2	−0.25	−0.25
30	−26.3	−0.14	−0.13	−45.4	−0.15	−0.12
40	−20.6	−0.09	−0.05	−35.0	−0.10	−0.04
50	−17.0	−0.06	0.00	−28.5	−0.07	−0.00

Note that approximating the solution of this equation for y by the inhomogeneous term causes ΔT to vanish, thus reproducing the convolution approximation. At small k, the integral term in (16) is proportional to k^2. Since $u(k)$ is negative, y will be predominantly negative, and thus also the integral term. Consequently $\Delta T < 0$.

Using Eq. (15), the Euler-Lagrange equation resulting from the self-consistent approximation is derived and analyzed precisely as in Ref. 1. The solutions will satisfy the perfect screening condition and appear to be otherwise well behaved.

Instead of actually solving this Euler-Lagrange equation, we took the simpler course of using the solutions from the convolution approximation Euler-Lagrange equation to evaluate the energy shift ΔT, Eq. (15). The results, shown in Table I, are of the order of a millirydberg or less, and are quite similar to the lowest-order HNC shifts obtained in Ref. 1. The table includes several values of the spin-degeneracy factor ν. $\nu=1$ corresponds to the completely polarized electron fluid, $\nu=2$ to the paramagnetic fluid, and $\nu=\infty$ to the charged boson fluid.

We conclude that the Clark-Westhaus expression for the kinetic energy with the convolution approximation is a very good approximation in the Coulomb fluid, comparable to the Jackson-Feenberg kinetic energy in the short-ranged systems.

ACKNOWLEDGMENTS

Research supported in part by the National Science Foundation and the Alexander von Humboldt Stiftung.

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[1]J. G. Zabolitzky, Phys. Rev. B 22, 2353 (1980), and references cited therein.

[2]C. E. Campbell, K. E. Kürten, and E. Krotscheck, Phys. Rev. B 25, 1633 (1982), and references cited therein.

[3]J. W. Clark, in *Progress in Particle and Nuclear Physics,* edited by D. H. Wilkinson (Pergamon, Oxford, 1979), Vol. II, and references cited therein.

[4]A similar transformation was used by M. Puoskari and A. Kallio, Phys. Scr. 24, 601 (1981).