

Nonlocal exchange energy of many-fermion systems of arbitrary dimensionality and interparticle interaction

G. Gumbs* and D. J. W. Geldart

Department of Physics, Dalhousie University, Halifax, Nova Scotia, Canada B3H 3J5

(Received 8 May 1986)

The exchange contributions to the ground-state energy of an inhomogeneous many-fermion system of arbitrary dimensionality are calculated. Explicit results are given for both the local-density approximation and the lowest-order gradient corrections for a class of interparticle interactions, including the Coulomb potential. For wider application, both the local-density approximation and the gradient corrections are decomposed into their wave-vector components. These exchange contributions can then be determined for arbitrary interparticle interaction by a simple quadrature.

I. INTRODUCTION

We give a gradient expansion representation for the ground-state exchange energy E_x as a functional of the electron density $n(\mathbf{r})$ for an inhomogeneous system of interacting fermions within a space of dimensionality d . Explicit forms are obtained for the coefficients $A_x(n)$ and $B_x(n)$ which determine the local-density approximation (LDA) and the lowest-order gradient corrections in

$$E_x[n] = \int d^d\mathbf{r} \{ A_x(n(\mathbf{r})) + B_x(n(\mathbf{r}))[\nabla n(\mathbf{r})]^2 + \dots \} . \tag{1}$$

The most immediate motivation for this work is the need for simple but reliable methods for calculating properties of quasi-two-dimensional electronic systems with microstructures. There are also other structures whose effective dimensionality is better described by a fractional or noninteger value of the dimensionality d . We shall not pursue this matter here but, for maximum generality, for systems with various force laws, we present results in a form which can be applied for arbitrary interparticle interaction $v(\mathbf{r})$. Explicit forms for $A_x(n)$ and $B_x(n)$ are also given for a class of power-law potentials, including the Coulomb potential ($1/r^{d-2}$), for arbitrary dimension d . The fourth-order density-gradient expansion for the ground-state fermion kinetic energy has recently been studied, with particular attention given to its convergence properties.¹ In that work, Eq. (1) was applied to a d -dimensional system of fermions coupled by Coulomb forces and having a model density profile simulating a vacuum-solid interface. In this paper, details of that calculation are presented and the formalism is extended considerably to obtain $A_x(n)$ and $B_x(n)$ for arbitrary interparticle interaction.

The paper is arranged as follows. In Sec. II, the lowest-order exchange contributions to the wave-vector-dependent polarizability in the ground-state energy is calculated for arbitrary interparticle interaction. In Sec. III, we evaluate the exchange contribution to the ground-state energy when the interparticle potential is assumed to be given by a pure power law in wave-vector space. Comments on some other cases are made. Section IV is devoted

to concluding remarks. A few details are given in the Appendix for a typical calculation involved in evaluating the polarization function.

II. GENERAL FORMULATION OF THE PROBLEM

The ground-state energy of an electron gas in the presence of an external potential $V(\mathbf{q})$ is given by second-order perturbation theory as

$$\Delta E_V \equiv E(V) - E(V=0) = \frac{1}{2} \sum_{\mathbf{q}} \tilde{n}(\mathbf{q}) V(\mathbf{q}) + O(V^3) , \tag{2}$$

where $\tilde{n}(\mathbf{q})$ is the induced electron density. With linear-response theory, $\tilde{n} = \Pi V \epsilon^{-1}$ where Π is the polarization and ϵ is the dielectric function. Thus Eq. (2) may be rewritten as

$$\Delta E_V = \sum_{\mathbf{q}} \tilde{n}(\mathbf{q}) V(\mathbf{q}) + \frac{1}{2} \sum_{\mathbf{q}} |\tilde{n}(\mathbf{q})|^2 [v(q) + \Pi^{-1}(\mathbf{q})] , \tag{3}$$

where $v(q)$ is the Fourier transform of the interparticle potential. The polarization is given by standard Feynman-graph expansion methods.² For noninteracting particles, the polarization is the usual Lindhard function. We are interested in lowest-order exchange corrections to the polarization. Explicit terms of first order in interparticle interactions are²

$$\Pi_A(\mathbf{q}) = 2 \text{tr}_{\mathbf{p}\zeta} \text{tr}_{\mathbf{p}'\zeta'} g_{\mathbf{p}}^0(\zeta) g_{\mathbf{p}+\mathbf{q}}^0(\zeta) v(\mathbf{p}-\mathbf{p}') g_{\mathbf{p}'}^0(\zeta') g_{\mathbf{p}'+\mathbf{q}}^0(\zeta') \tag{4a}$$

and

$$\begin{aligned} \Pi_B^{(1)}(\mathbf{q}) &= 2 \text{tr}_{\mathbf{p}\zeta} \text{tr}_{\mathbf{p}'\zeta'} \\ &\times [g_{\mathbf{p}}^0(\zeta)^2 g_{\mathbf{p}+\mathbf{q}}^0(\zeta) v(\mathbf{p}-\mathbf{p}') g_{\mathbf{p}'}^0(\zeta') \\ &+ g_{\mathbf{p}}^0(\zeta) g_{\mathbf{p}+\mathbf{q}}^0(\zeta)^2 v(\mathbf{p}-\mathbf{p}') g_{\mathbf{p}'+\mathbf{q}}^0(\zeta')] , \end{aligned} \tag{4b}$$

which correspond to vertex and self-energy corrections, respectively, and could be expressed in terms of the exchange self-energy

$$\Sigma_x(\mathbf{p}) = -\text{tr}_{\mathbf{p}'\zeta} v(\mathbf{p}-\mathbf{p}') g_{\mathbf{p}}^0(\zeta') e^{\zeta_0^+}. \quad (5)$$

$g_{\mathbf{p}}^0(\zeta)$ is the Green's function for a noninteracting system, ζ is a continuous "frequency" variable corresponding to the $T \rightarrow 0$ limit of Matsubara frequencies ζ_n and

$$\text{tr}_{\mathbf{p}\zeta}(\dots) = \sum_{\zeta_n} \int \frac{d^d \mathbf{p}}{(2\pi)^d} (\dots). \quad (6)$$

In addition, there is also a contribution due to the implicit dependence of the chemical potential on interactions. The Green's function is given by

$$g_{\mathbf{p}}(\zeta) = \frac{1}{\zeta + \mu - \epsilon_{\mathbf{p}}}, \quad (7)$$

where the chemical potential μ for the interacting system is related to that for the noninteracting system μ_0 (at $T=0$) by³

$$\mu - \mu_0 \equiv \delta\mu = \Sigma_x(k_F). \quad (8)$$

k_F is the Fermi momentum. This gives the final contribution of first order in the interaction

$$\Pi_B^{(2)}(\mathbf{q}) = \delta\mu \frac{\partial}{\partial \mu_0} \Pi_0(\mathbf{q}), \quad (9)$$

where

$$\Pi_0(\mathbf{q}) = -2 \text{tr}_{\mathbf{p}\zeta} g_{\mathbf{p}}^0(\zeta) g_{\mathbf{p}+\mathbf{q}}^0(\zeta). \quad (10)$$

Expanding in powers of q^2 , the various contributions to the polarization are obtained by expanding individual propagators in powers of \mathbf{q} , evaluating angular integrations and collecting results. We obtain

$$\Pi_0(q) = 2K_d m k_F^{d-4} [k_F^2 - \frac{1}{12}(d-2)q^2] \quad (11)$$

and

$$\Pi_B^{(2)}(q) = 2\delta\mu K_d m^2 (d-2) k_F^{d-6} [k_F^2 - \frac{1}{12}(d-4)q^2], \quad (12)$$

where m is the electron mass, $K_d = \Omega_d / (2\pi)^d$ and $\Omega_d = 2\pi^{d/2} / \Gamma(d/2)$. For maximum generality, we carry through the analysis for arbitrary electron-electron interaction as far as possible.

It is convenient to combine Π_A and $\Pi_B^{(1)}$, rather than calculate them separately. Setting $\Pi_A(\mathbf{q}) = \Pi_A(0) + \delta\Pi_A(\mathbf{q})$ and $\Pi_B^{(1)}(\mathbf{q}) = \Pi_B^{(1)}(0) + \delta\Pi_B^{(1)}(\mathbf{q})$, we have

$$\begin{aligned} \Pi_A(0) + \Pi_B^{(1)}(0) &= 2 \frac{\partial}{\partial \mu_0} \text{tr}_{\mathbf{p}} \text{tr}_{\mathbf{p}'} \delta(\mu_0 - \epsilon_{\mathbf{p}'}) \\ &\quad \times v(\mathbf{p}-\mathbf{p}') \eta_+(\mu_0 - \epsilon_{\mathbf{p}'}), \end{aligned} \quad (13a)$$

$$\begin{aligned} \delta\Pi_A(\mathbf{q}) + \delta\Pi_B^{(1)}(\mathbf{q}) &= \frac{1}{2m} q^2 \left[\frac{\partial}{\partial \mu_0} \left(I_1 + \frac{2}{3d} I_3 \right) + \frac{1}{3} I_2 \right]. \end{aligned} \quad (13b)$$

Here $\eta_+(x)$ is the Heaviside unit step function and

$$I_1 = -\frac{\partial}{\partial \mu_0} \text{tr}_{\mathbf{k}} v(\mathbf{k}) A_{\mathbf{k}} + \text{tr}_{\mathbf{k}} v(\mathbf{k}) B_{\mathbf{k}}, \quad (14a)$$

$$I_2 = \frac{\partial^2}{\partial \mu_0^2} \text{tr}_{\mathbf{k}} v(\mathbf{k}) A_{\mathbf{k}} - \frac{3}{2} \frac{\partial}{\partial \mu_0} \text{tr}_{\mathbf{k}} v(\mathbf{k}) B_{\mathbf{k}}, \quad (14b)$$

$$\begin{aligned} I_3 &= \frac{\partial^2}{\partial \mu_0^2} \text{tr}_{\mathbf{k}} v(\mathbf{k}) C_{\mathbf{k}} - \frac{3}{2} \frac{\partial}{\partial \mu_0} \text{tr}_{\mathbf{k}} v(\mathbf{k}) D_{\mathbf{k}} \\ &\quad - \frac{1}{4} \frac{\partial}{\partial \mu_0} \text{tr}_{\mathbf{k}} v(\mathbf{k}) \epsilon_{\mathbf{k}} B_{\mathbf{k}} - \frac{1}{2} \text{tr}_{\mathbf{k}} v(\mathbf{k}) F_{\mathbf{k}}, \end{aligned} \quad (14c)$$

where $[f(\tilde{\epsilon}_{\mathbf{p}})]$ is the Fermi distribution function and $\tilde{\epsilon}_{\mathbf{p}} = \epsilon_{\mathbf{p}} - \mu_0$

$$\begin{aligned} A_{\mathbf{k}} &\equiv \text{tr}_{\mathbf{p}} (\tilde{\epsilon}_{\mathbf{p}+\mathbf{k}}) \frac{\partial f(\tilde{\epsilon}_{\mathbf{p}})}{\partial \mu_0} \\ &= \frac{\Omega_{d-1}}{(2\pi)^d} \frac{2^{d-1}}{d-1} \left[\frac{2k_F - k}{4k_F} \right]^{(d-1)/2} m k_F^{d-2} \eta_+(2k_F - k) F \left[\frac{d-1}{2}, \frac{3-d}{2}, \frac{d+1}{2}, \frac{2k_F - k}{4k_F} \right], \end{aligned} \quad (15a)$$

$$\begin{aligned} B_{\mathbf{k}} &\equiv \text{tr}_{\mathbf{p}} \frac{\partial f(\tilde{\epsilon}_{\mathbf{p}+\mathbf{k}})}{\partial \mu_0} \frac{\partial f(\tilde{\epsilon}_{\mathbf{p}})}{\partial \mu_0} \\ &= \frac{1}{2} \frac{\Omega_{d-1}}{(2\pi)^d} m^2 k_F^{d-3} \left[1 - \left[\frac{k}{2k_F} \right]^2 \right]^{(d-3)/2} \eta_+(2k_F - k), \end{aligned} \quad (15b)$$

$$\begin{aligned} C_{\mathbf{k}} &\equiv \text{tr}_{\mathbf{p}} \epsilon_{\mathbf{p}} f(\tilde{\epsilon}_{\mathbf{p}+\mathbf{k}}) \frac{\partial f(\tilde{\epsilon}_{\mathbf{p}})}{\partial \mu_0} \\ &= \frac{\Omega_{d-1}}{(2\pi)^d} \frac{2^{d-2}}{d-1} \left[\frac{2k_F - k}{4k_F} \right]^{(d-1)/2} k_F^d \eta_+(2k_F - k) F \left[\frac{d-1}{2}, \frac{3-d}{2}, \frac{d+1}{2}, \frac{2k_F - k}{4k_F} \right], \end{aligned} \quad (15c)$$

$$\begin{aligned} D_{\mathbf{k}} &\equiv \text{tr}_{\mathbf{p}} \epsilon_{\mathbf{p}} \frac{\partial f(\tilde{\epsilon}_{\mathbf{p}+\mathbf{k}})}{\partial \mu_0} \frac{\partial f(\tilde{\epsilon}_{\mathbf{p}})}{\partial \mu_0} \\ &= \frac{1}{4k} \frac{\Omega_{d-1}}{(2\pi)^d} m k_F^{d-1} \left[1 - \left[\frac{k}{2k_F} \right]^2 \right]^{(d-3)/2} \eta_+(2k_F - k), \end{aligned} \quad (15d)$$

$$\begin{aligned}
F_{\mathbf{k}} &\equiv \frac{1}{m} \text{tr}_{\mathbf{p}} \mathbf{p} \cdot \mathbf{k} \frac{\partial^2 f(\tilde{\epsilon}_{\mathbf{p}+\mathbf{k}})}{\partial \mu_0^2} \frac{\partial f(\tilde{\epsilon}_{\mathbf{p}})}{\partial \mu_0} \\
&= -\frac{1}{2} \frac{\Omega_{d-1}}{(2\pi)^d} m k_F^{d-2} \left\{ \frac{1}{4} (d-3) m \frac{k}{k_F^3} \left[1 - \left(\frac{k}{2k_F} \right)^2 \right]^{(d-5)/2} \eta_+(2k_F-k) \right. \\
&\quad \left. - \frac{m}{kk_F} \left[1 - \left(\frac{k}{2k_F} \right)^2 \right]^{(d-3)/2} \eta_+(2k_F-k) \right. \\
&\quad \left. + \frac{k}{2k_F} \left[1 - \left(\frac{k}{2k_F} \right)^2 \right]^{(d-3)/2} \delta \left[\frac{k(2k_F-k)}{2m} \right] \right\}. \tag{15e}
\end{aligned}$$

In Eqs. (15), $F(a, b; c; z)$ is a hypergeometric function and, after appropriate reductions, the required integrals may be obtained in a straightforward way with the use of standard tables.⁴ In the Appendix $A_{\mathbf{k}}$ is calculated explicitly and the other functions in Eqs. (15b)–(15e) may be obtained in a similar way. In Sec. III we calculate the exchange energy through second-order gradients of the electron density for a pure power-law interparticle potential. The results presented in Ref. 1 are a special case corresponding to the Coulomb potential $v(k) \sim k^{-2}$.

III. THE GRADIENT EXPANSION FOR THE EXCHANGE ENERGY FOR PURE POWER-LAW INTERPARTICLE POTENTIAL

In this section we apply the results presented in Sec. II for $v(k) = Q_d k^{-2\eta}$, where the power-law exponent 2η is arbitrary and $Q_d \equiv e^2 \Omega_d$. In a straightforward way it may be shown that

$$\delta\mu = -\frac{1}{d} K_d Q_d k_F^{d-2\eta} \frac{\Gamma\left(\frac{d}{2}+1\right) \Gamma(d-2\eta)}{\Gamma\left(\frac{d}{2}+1-\eta\right) \Gamma(d-\eta)} \tag{16}$$

and

$$\begin{aligned}
\Pi_A(0) + \Pi_B^{(1)}(0) &= \frac{4}{d} m^2 (d-1-\eta) K_d^2 Q_d k_F^{2(d-2-\eta)} \\
&\quad \times F\left[\eta, \eta+1 - \frac{d}{2}; \frac{d}{2}+1; 1\right]. \tag{17}
\end{aligned}$$

Denoting the expansion of the polarization as

$$\Pi(\mathbf{q}) = a^{-1} - b q^2 + O(q^4), \tag{18}$$

the coefficients a and b can be identified from the results of our calculations. Equations (11), (12), (16), and (17) jointly give a^{-1} which in turn yields

$$\begin{aligned}
a &= \frac{1}{2m K_d k_F^{d-2}} \left[1 - \frac{m}{d} (d-2\eta) K_d Q_d k_F^{d-2-2\eta} \right. \\
&\quad \left. \times F\left[\eta, \eta+1 - \frac{d}{2}; \frac{d}{2}+1; 1\right] \right]. \tag{19}
\end{aligned}$$

Equation (19) yields the LDA for the kinetic energy and exchange energy as

$$T_{\text{LDA}}[n] = \frac{1}{2m} \left[\frac{d}{2K_d} \right]^{2/d} \left[\frac{d}{2+d} \right] \int d\mathbf{r} n^{(d+2)/d}(\mathbf{r}), \tag{20a}$$

$$E_x^{\text{LDA}}[n] = -\frac{1}{4} Q_d \left[\frac{2K_d}{d} \right]^{2\eta/d} \left[\frac{d}{d-\eta} \right] F\left[\eta, \eta+1 - \frac{d}{2}; \frac{d}{2}+1; 1\right] \int d\mathbf{r} n^{2(d-\eta)/d}(\mathbf{r}). \tag{20b}$$

Turning now to the quantities I_1 , I_2 , and I_3 in Eqs. (14), we obtain

$$\begin{aligned}
I_1 &= -\frac{\Omega_{d-1}}{(2\pi)^d} K_d Q_d m^2 k_F^{2(d-2-\eta)} 2^{d-2\eta-3} \\
&\quad \times \left[2^{(d+7)/2} \left[\frac{d-1-\eta}{d-1} \right] B\left[\frac{d+1}{2}, d-2\eta\right] F\left[\frac{d-1}{2}, \frac{3-d}{2}; \frac{3d+1-4\eta}{2}; \frac{1}{2}\right] - B\left[\frac{d-1-2\eta}{2}, \frac{d-1}{2}\right] \right], \tag{21}
\end{aligned}$$

$$I_2 = \frac{\Omega_{d-1}}{(2\pi)^d} K_d Q_d m^3 k_F^{2(d-3-\eta)} (d-2-\eta) 2^{d-3-2\eta} \times \left[2^{(d+9)/2} \left[\frac{d-1-\eta}{d-1} \right] B \left[\frac{d+1}{2}, d-2\eta \right] F \left[\frac{d-1}{2}, \frac{3-d}{2}; \frac{3d+1-4\eta}{2}; \frac{1}{2} \right] - 3B \left[\frac{d-1-2\eta}{2}, \frac{d-1}{2} \right] \right], \quad (22)$$

$$I_3 = \frac{\Omega_{d-1}}{(2\pi)^d} K_d Q_d m^2 k_F^{2(d-2-\eta)} \times \left[\frac{(d-\eta)(d-\eta-1)}{d-1} 2^{(3d-4\eta+1)/2} B \left[\frac{d+1}{2}, d-2\eta \right] \times F \left[\frac{d-1}{2}, \frac{3-d}{2}; \frac{3d+1-4\eta}{2}; \frac{1}{2} \right] - 3(d-\eta-1) 2^{d-4-2\eta} B \left[\frac{d-1-2\eta}{2}, \frac{d-1}{2} \right] - (d-\eta-1) 2^{d-2\eta-3} B \left[\frac{d+1-2\eta}{2}, \frac{d-1}{2} \right] + (d-3) 2^{d-2\eta-4} B \left[\frac{d+1-2\eta}{2}, \frac{d-3}{2} \right] - 2^{d-2\eta-4} B \left[\frac{d-1-2\eta}{2}, \frac{d-1}{2} \right] \right]. \quad (23)$$

We obtain the results for the k^{-2} Coulomb potential for which explicit results were presented in Ref. 1, by setting $\eta=1$ in Eqs. (21)–(23). We have

$$I_1(\eta=1) = -Q_d K_d^2 m^2 k_F^{2(d-3)} \frac{3d-10}{4(d-3)}, \quad (24)$$

$$I_2(\eta=1) = \frac{1}{4} Q_d K_d^2 m^3 k_F^{2(d-4)} (5d-18), \quad (25)$$

$$I_3(\eta=1) = \frac{1}{2} Q_d K_d^2 m^2 k_F^{2(d-3)} \left[2(d-1) - \frac{1}{4} \frac{(d-2)(3d-5)}{d-3} \right]. \quad (26)$$

Collecting results for $\Pi(\mathbf{q})$, we obtain the wave-vector-dependent contribution for the polarization to order q^2 . We have

$$-bq^2 = \epsilon_q \left[-\frac{1}{3} K_d m^2 (d-2) k_F^{d-4} - \frac{1}{3} \delta\mu K_d m^3 (d-2)(d-4) k_F^{d-6} + Q_d K_d^2 m^3 k_F^{2(d-3-\eta)} R_d \right], \quad (27)$$

where

$$\frac{\partial}{\partial\mu_0} \left[I_1 + \frac{2}{3d} I_3 \right] + \frac{1}{3} I_2 = K_d^2 Q_d m^3 k_F^{2(d-3-\eta)} R_d \quad (28)$$

with R_d defined by the equation

$$R_d = \frac{2^{d-2\eta-2}}{B \left[\frac{d-1}{2}, \frac{1}{2} \right]} \frac{(d-2-\eta)}{3d} \left[-2^{(d+9)/2} \eta \frac{(d-1-\eta)}{d-1} B \left[\frac{d+1}{2}, d-2\eta \right] F \left[\frac{d-1}{2}, \frac{3-d}{2}; \frac{3d+1-4\eta}{2}; \frac{1}{2} \right] + \frac{1}{2} (6\eta+4-3d) B \left[\frac{d-1-2\eta}{2}, \frac{d-1}{2} \right] - \frac{1}{2} (d-1-\eta) B \left[\frac{d+1-2\eta}{2}, \frac{d-1}{2} \right] + (d-3) B \left[\frac{d+1-2\eta}{2}, \frac{d-3}{2} \right] \right]. \quad (29)$$

The second-order gradient terms for the kinetic and exchange energies are therefore

$$T_2[n] = \frac{1}{2m} \left[\frac{d-2}{12d} \right] \int d\mathbf{r} \frac{(\nabla n)^2}{n} \quad (30)$$

and

$$E_x^{(2)}[n] = \frac{1}{2} v_d \int d\mathbf{r} \frac{(\nabla n)^2}{n^{2(1+\eta)d}}, \quad (31)$$

where

$$v_d = -\frac{1}{24d} Q_d \left(\frac{2K_d}{d} \right)^{2(1+\eta)/d} \times \left[3dR_d + (d-2)(3d-4-4\eta) \right. \\ \left. \times \frac{\Gamma\left(\frac{d}{2}+1\right)\Gamma(d-2\eta)}{\Gamma\left(\frac{d}{2}+1-\eta\right)\Gamma(d-\eta)} \right]. \quad (32)$$

It is a simple matter to show that when $\eta=1$, we obtain

$$R_d(\eta=1) = \frac{1}{12d}(28-3d^2) \quad (33)$$

and

$$v_d(\eta=1) = \frac{1}{96d} Q_d \left(\frac{2K_d}{d} \right)^{4/d} (3d^2 - 16d + 28), \quad (34)$$

which agrees with the results presented in Ref. 1 which were carried out specifically for a $1/k^2$ potential.

Setting $d=2$ in Eq. (29), we obtain

$$R_{d=2} = \frac{1}{3} \eta 2^{-4\eta} \left[\eta(1-\eta) 2^{4\eta+1} \frac{\Gamma(2-2\eta)}{[\Gamma(2-\eta)]^2} \right. \\ \left. - (11-21\eta) \frac{\Gamma(1-2\eta)}{[\Gamma(1-\eta)]^2} \right]. \quad (35)$$

Of course, the second term in Eq. (32) does not contribute when we set $d=2$ and allow η to be arbitrary. Equations (32) and (35) jointly give

$$v_{d=2}(\eta=1) = -\frac{1}{24} Q_2 K_2^2, \quad (36)$$

which is consistent with Eq. (34) when $d=2$. This may appear slightly surprising at first when one finds that R_d in Eq. (33) at $d=2$ is twice the value obtained from Eq. (35) when η is set equal to unity. This apparent discrepancy is due to the order in which the limits $d \rightarrow 2$ and $\eta \rightarrow 1$ are taken near the singularities in the Γ functions in Eqs. (29) and (32). There is a factor in R_d which varies as $(d-1-\eta)/(d-2\eta)$ for $d \approx 2$ and $\eta \approx 1$ which takes on the value $\frac{1}{2}$ if $d \rightarrow 2$ before $\eta \rightarrow 1$, and the value 1 if $\eta \rightarrow 1$ before $d \rightarrow 2$. However, there is also a singular factor in the second term on the right-hand side of Eq. (32) of the form $(d-2)/(d-2\eta)$. When both terms are taken care of correctly, it is seen that v_d of Eq. (32) is regular near $d=2$ and $\eta=1$. From a physical point of view, we expect v_d and all other coefficients in the gradient expansion, if they are finite, would have a unique value,

whatever may be the order in which d and η are chosen.

The value of $\eta = \frac{1}{2}$ may be of some interest in studies of a quasi-two-dimensional electron gas since $2\pi e^2/k$ is the two-dimensional Fourier transform of e^2/r ,

$$\frac{2\pi e^2}{k} = \lim_{\lambda \rightarrow 0} \int d^2r e^{-ik \cdot r} \frac{e^{-\lambda r}}{r}. \quad (37)$$

A pure power law is an idealization, of course, and taking proper account of the structure of quasi-two-dimensional devices leads to a much more complicated k dependence.⁵ Disregarding this here, we set $\eta = \frac{1}{2}$ in Eq. (32) and see that v_d for this case has a singularity varying as $1/(d-2)$ for d near 2. However, this singularity is spurious and is removed when the finite structure of physical devices is taken into account (e.g., the finite thickness of oxide layers). The general formulation of Sec. II is then both necessary and sufficient for dealing with this situation as it is not limited to pure power laws.

IV. SUMMARY

We have calculated the coefficients in the gradient expansion for the kinetic energy and the lowest-order exchange energy for an interacting many-fermion system in its ground state. This spatial dimensionality and the precise form of the interparticle interaction have been kept arbitrary in the general formulation and results for any given interparticle interaction are obtainable by elementary quadrature. Analytical results have been given for the case of a pure power law, $k^{-2\eta}$ in wave-number space, for the interparticle interaction. In some cases, such as quasi-two-dimensional electron systems, care is required in specifying the interparticle interaction and the general wave-vector decomposition is required for a proper treatment of systems which are not fully describable by pure power laws.

Gradient expansions for the kinetic energy can be obtained from the Wigner-Kirkwood partition function. The gradient expansion for the exchange energy of a three-dimensional electron gas has also been discussed by Gross and Dreizler⁶ using Kirzhnits's expansion of the density matrix. The present method of calculation, based on long-wavelength expansions of the irreducible part of the density-density correlation function is very convenient and is easily generalized to include higher-order correlation effects. We hope to report results for extensions and applications elsewhere.

ACKNOWLEDGMENTS

Financial support from the Natural Sciences and Engineering Research Council (NSERC) of Canada is gratefully acknowledged. One of us (G.G) also thanks NSERC for additional financial support.

APPENDIX

In this appendix we evaluate A_k defined in Eq. (15), at $T=0$. In a straightforward way we obtain

$$\begin{aligned}
 A_{\mathbf{k}} &\equiv \text{tr}_{\mathbf{p}} f(\tilde{\epsilon}_{\mathbf{p}+\mathbf{k}}) \frac{\partial f(\tilde{\epsilon}_{\mathbf{p}})}{\partial \mu_0} \\
 &= \frac{\Omega_{d-1}}{(2\pi)^d} \int_0^\infty dp p^{d-1} \frac{\partial f(\tilde{\epsilon}_{\mathbf{p}})}{\partial \mu_0} \int_0^\pi d\theta (\sin\theta)^{d-2} \int_{-\infty}^\infty dy f(y) \delta \left[\mu_0 + y - \frac{1}{2m} (p^2 + 2pk \cos\theta + k^2) \right].
 \end{aligned}
 \tag{A1}$$

Integrating over θ , Eq. (A1) becomes

$$\begin{aligned}
 A_{\mathbf{k}} &= \left[\frac{m}{k} \right]^{d-2} \frac{\Omega_{d-1}}{(2\pi)^d} \\
 &\times \int_0^\infty dp p \frac{\partial f(\tilde{\epsilon}_{\mathbf{p}})}{\partial \mu_0} \\
 &\times \int_{y_{\min}}^{y_{\max}} dy f(y) (y_{\max} - y)^{(d-3)/2} \\
 &\times (y - y_{\min})^{(d-3)/2},
 \end{aligned}
 \tag{A2}$$

where

$$y_{\min} \equiv \frac{1}{2m} (p - k)^2 - \mu_0, \tag{A3a}$$

$$y_{\max} \equiv \frac{1}{2m} (p + k)^2 - \mu_0. \tag{A3b}$$

It is a simple matter to evaluate the y integral in Eq. (A2) at $T=0$ with $f(y) = \eta_+(-y)$. After a little algebra, we obtain

$$\begin{aligned}
 A_{\mathbf{k}} &= \frac{\Omega_{d-1}}{(2\pi)^d} \frac{2^{d-1}}{d-1} \\
 &\times \int_0^\infty dp p^{d-1} \frac{\partial f(\tilde{\epsilon}_{\mathbf{p}})}{\partial \mu_0} \eta_+(s_0) \\
 &\times \eta_+(1-s_0) s_0^{(d-1)/2} \\
 &\times F \left[\frac{d-1}{2}, \frac{3-d}{2}; \frac{d+1}{2}; s_0 \right],
 \end{aligned}
 \tag{A4}$$

where $s_0 \equiv (2k_F - k)/4k_F$. Equation (A4) readily yields the result in Eq. (15) for $A_{\mathbf{k}}$. In Eq. (A4), $F(a, b; c; z)$ denotes the usual hypergeometric function [also often denoted by ${}_2F_1(a, b; c; z)$]. The remaining quantities $B_{\mathbf{k}}$, $C_{\mathbf{k}}$, $D_{\mathbf{k}}$, and $F_{\mathbf{k}}$ in Eq. (14) are obtained analogously.

*Present address: Department of Physics, University of Lethbridge, Lethbridge, Alberta, Canada T1K 3M4.

¹D. J. W. Geldart and G. Gumbs, Phys. Rev. B 33, 2820 (1986).

²We follow closely the notation and procedures of D. J. W. Geldart and M. Rasolt, Phys. Rev. B 13, 1477 (1976). References to earlier work are also given there.

³J. M. Luttinger and J. C. Ward, Phys. Rev. 118, 1417 (1960).

⁴I. S. Gradshteyn and I. M. Ryzhik, *Tables of Integrals, Series and Products* (Academic, New York, 1965).

⁵A. V. Chaplik, Zh. Eksp. Teor. Fiz. 62, 746 (1972) [Sov. Phys.—JETP 35, 395 (1972)].

⁶E. K. U. Gross and R. M. Dreizler, Z. Phys. A 302, 103 (1981).