Kirzhnits gradient expansion in two dimensions

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We derive the semiclassical Kirzhnits expansion of the D-dimensional one-particle density matrix up to the second order in $\hbar$. We focus on the two-dimensional (2D) case and show that all the gradient corrections both to the 2D one-particle density and to the kinetic energy vanish. However, the 2D Kirzhnits expansion satisfies the consistency criterion of Gross and Proetto [J. Chem. Theory Comput. **5**, 844 (2009)] for the functional derivatives of the density and the noninteracting kinetic energy with respect to the Kohn-Sham potential. Finally, we show that the gradient correction to the exchange energy diverges in agreement with the previous linear-response study.

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I. INTRODUCTION

Gradient expansions provide a natural path to correct the local-density approximation (LDA) for slowly-varying densities as already suggested by Hohenberg and Kohn in their seminal paper on density-functional theory[1] (DFT). The second-order gradient expansion for the kinetic energy was shown to be very useful, but on the other hand, systematic gradient expansions for the exchange and particularly for the correlation energies faced problems that were later corrected—at least from the practical viewpoint—by generalized-gradient approximations[2] (GGAs). Nevertheless, gradient expansions pose still open questions, especially in reduced dimensions such as the two-dimensional electron gas[3] (2DEG). The interest in the 2DEG arises from a multitude of applications in, e.g., quantum Hall and semiconductor physics.

Semiclassical gradient expansions can be regarded as alternatives to the standard approaches based on Taylor expansions and linear-response formalism. Although semiclassical methods do not give access to the correlation energy, they can be used to derive simple density functionals for the Kohn-Sham (KS) kinetic energy T_s and the exchange energy density ϵ_x (Ref. 4). Here we focus on the semiclassical Kirzhnits commutator formalism.[5] It has been previously used to derive the lowest-order (second order in $\hbar$) gradient correction terms to the one-particle density matrix $\gamma(\mathbf{r},\mathbf{r}')$ and to ϵ_x in three dimensions (3D),[6] as well as for T_s in D dimensions.[7] Higher-order corrections in 3D have been analyzed in Ref. 8.

In this paper we use the Kirzhnits method to derive the lowest-order gradient corrections to the one-particle density matrix in D dimensions. Then we focus on the 2D case and show that all the corrections to the one-particle density $n(\mathbf{r})$ vanish, and, in agreement with Refs. 7 and 9–11, they vanish also for T_s. Due to the resulting simple expressions for $n(\mathbf{r})$ and T_s, the consistency criterion of Gross and Proetto[12] that couples the functional derivatives of T_s and $n(\mathbf{r})$ is satisfied. Finally, we show that the gradient corrections to ϵ_x *diverge* in the 2D Kirtzhnits expansion, which is in agreement with the linear-response results of Gumbs and Geldart.[13]

II. KIRZHNITS EXPANSION IN D DIMENSIONS

The exchange energy E_x and the KS kinetic energy T_s can be expressed as[4,14]

$$E_x = -\frac{1}{4}\int d^D r\, d^D r' \frac{|\gamma(\mathbf{r},\mathbf{r}')|^2}{|\mathbf{r}-\mathbf{r}'|} \qquad (1)$$

$$T_s = -\frac{\hbar^2}{2m}\int d^D r \left\{\nabla^2_{\mathbf{r}}\gamma(\mathbf{r},\mathbf{r}')\right\}_{\mathbf{r}'=\mathbf{r}}, \qquad (2)$$

where the one-particle density matrix can be written in terms of the Fermi energy ϵ_F as

$$\begin{aligned}\gamma(\mathbf{r},\mathbf{r}') &= \sum_{j:\epsilon_j\leqslant\epsilon_F}\varphi_j^*(\mathbf{r})\varphi_j(\mathbf{r}') \\ &= \sum_j \Theta(\epsilon_F-\epsilon_j)\varphi_j^*(\mathbf{r})\varphi_j(\mathbf{r}') \\ &= \langle\mathbf{r}|\Theta(\epsilon_F-\hat{t}-\hat{v}_S)|\mathbf{r}'\rangle. \end{aligned} \qquad (3)$$

Here Θ_i are the solutions of the single-particle KS equation, $\hat{t}$ is the kinetic energy operator, $\hat{v}_s$ is the KS potential, and Θ is the Heaviside step function. Now we define the local Fermi energy $\hat{E}_F(\mathbf{r}) \equiv \epsilon_F - v_s(\mathbf{r})$ and use the plane-wave decomposition as

$$\gamma(\mathbf{r},\mathbf{r}') = \sum_{\alpha=\pm}\int d^D k \langle\mathbf{r}|\Theta(\hat{E}_F-\hat{t})|\mathbf{k}\alpha\rangle\langle\mathbf{k}\alpha|\mathbf{r}'\rangle, \qquad (4)$$

where $|\mathbf{k}\alpha\rangle$ (with α as the spin index) are eigenfunctions of the momentum operator $\hat{p}$.

We introduce the abbreviated notations: $\Theta(\hat{E}_F-\hat{t}) = f(\hat{a}+\hat{b})$, $f=\Theta$, $\hat{a} = -\hat{t} = -\hat{p}^2/2$, and $\hat{b} = \hat{E}_F = \hat{k}_F^2/2$. Now we can use the inverse Laplace transform, the Fourier-Mellin integral, to show that the operator $\Theta(\hat{E}_F-\hat{t})$ acts on eigenfunctions $|\mathbf{k}\rangle$ as

$$\begin{aligned} f(\hat{a}+\hat{b})|a\rangle &= \mathcal{L}^{-1}\{F(\beta)\}|a\rangle \\ &= \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} d\beta\, F(\beta)e^{\beta(\hat{a}+\hat{b})}|a\rangle, \end{aligned} \qquad (5)$$

where $c = \mathrm{Re}(\beta) > 0$ is arbitrary, but chosen such that the contour path of the integration is in the region of convergence of $F(\beta)$. The commutation problem of operators $\hat{a}$ and $\hat{b}$ can be avoided by introducing a new operator $\hat{K}(\beta)$ (see Refs. 4

and 8) such that

$$e^{\beta(\hat{a}+\hat{b})} = e^{\beta\hat{b}}\hat{K}(\beta)e^{\beta\hat{a}}. \tag{6}$$

Thus, we obtain for Eq. (5) an expression

$$f(\hat{a}+\hat{b})|a\rangle = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} d\beta\, F(\beta)e^{\beta(a+\hat{b})}\hat{K}(\beta)|a\rangle, \tag{7}$$

where the operator $\hat{a}$ has now been replaced with eigenvalue a in the exponential function, so that it commutes with the operator $\hat{b}$.

The expression for the operator $\hat{K}(\beta)$ is obtained by expanding it in a power series with respect to β,

$$\hat{K}(\beta) = \sum_{n=0}^{\infty}\beta^n\hat{O}_n. \tag{8}$$

Differentiating both sides of Eq. (6) with respect to β, and expanding all exponential functions in a Taylor series, leads to the recurrence relation[4,8]

$$\hat{O}_0 = 1, \qquad \hat{O}_1 = 0, \tag{9}$$

$$\hat{O}_{n+1} = \frac{1}{n+1}\left([\hat{a},\hat{O}_n] + \sum_{j=1}^{n}\hat{G}_j\hat{O}_{n-j}\right) \tag{10}$$

$$\hat{G}_j = \tfrac{(-1)^j}{j!}\underbrace{[\hat{b},[\hat{b},[\ldots[\hat{b}}_{j\text{times}},\hat{a}]\ldots]. \tag{11}$$

Inserting Eq. (8) in Eq. (5) yields

$$f(\hat{a}+\hat{b})|a\rangle = \sum_{n=0}^{\infty}\left[\frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} d\beta\, F(\beta)\beta^n e^{\beta(a+\hat{b})}\right]\hat{O}_n|a\rangle$$
$$= \sum_{n=0}^{\infty} f^{(n)}(a+\hat{b})\hat{O}_n|a\rangle, \tag{12}$$

where $f^{(n)}$ is the nth derivative of the function f. The Kirzhnits expansion in Eq. (12) leads to the following expression of the density matrix,

$$\gamma(\mathbf{r},\mathbf{r}') = \underbrace{\sum_{\alpha=\pm}\int d^Dk\,\Theta\left(E_F - \frac{k^2}{2}\right)\langle\mathbf{r}|\mathbf{k}\alpha\rangle\langle\mathbf{k}\alpha|\mathbf{r}'\rangle}_{\gamma^{(0)}}$$
$$+\sum_{n=2}^{\infty}\sum_{\alpha=\pm}\int d^Dk\,\delta^{(n-1)}\left[E_F - \frac{k^2}{2}\right]$$
$$\times\langle\mathbf{r}|\hat{O}_n|\mathbf{k}\alpha\rangle\langle\mathbf{k}\alpha|\mathbf{r}'\rangle, \tag{13}$$

where $\delta^{(n)}$ is the nth derivative of the delta function. The first term of Eq. (13), $\gamma^{(0)}$, corresponds to the zeroth order solution of the one-particle density matrix, and it can be written as

$$\gamma^{(0)}(\mathbf{r},\mathbf{r}') = \sum_{\alpha=\pm}\int d^Dk\,\Theta\left(E_F - \frac{\hbar^2k^2}{2m}\right)\langle\mathbf{r}|\mathbf{k}\alpha\rangle\langle\mathbf{k}\alpha|\mathbf{r}'\rangle$$
$$= \frac{2\delta_{\sigma,\sigma'}}{(2\pi)^D}\int_0^{k_F} dk\,k^{D-1}I(ky), \tag{14}$$

where $I(ky)$ is the $(D-1)$-dimensional surface integral given by

$$I(ky) \equiv \int d\Omega_{D-1}e^{iky\cos\theta}$$
$$= (2\pi)^{\frac{D}{2}}(ky)^{1-\frac{D}{2}}J_{\frac{D}{2}-1}(ky), \quad D \geqslant 2. \tag{15}$$

Here θ is the angle between vectors $\mathbf{y} = \mathbf{r} - \mathbf{r}'$ and $\mathbf{k}$, and $J_n(z)$ is the Bessel function of the first kind in order n. Thus we find an expression

$$\gamma^{(0)}(\mathbf{r},y) = \frac{2\delta_{\sigma,\sigma'}}{(2\pi)^{\frac{D}{2}}}k_F^D z^{-D/2}J_{\frac{D}{2}}(z), \tag{16}$$

where we use a definition $z = z(\mathbf{r},y) = k_F(\mathbf{r})|\mathbf{y}|$. This term generates the exact exchange energy for the homogeneous electron gas, which can be used as the LDA in an inhomogeneous system.

Higher-order terms of the Kirzhnits expansion $\gamma^{(n)}$ can be determined by calculating higher derivatives of the delta function and multiple commutators of $\hat{E}_F$ and $\hat{t}$ that lead to multiple derivatives of k_F. The intermediate steps in the calculation of the second-order (∇^2) inhomogeneity correction $\gamma^{(2)}(\mathbf{r},\mathbf{r}')$ are given in the Appendix. Combining our results leads to the semiclassical expansion of the density matrix of the form

$$\gamma(\mathbf{r},\mathbf{r}') = \gamma^{(0)}(\mathbf{r},\mathbf{r}') + \gamma^{(2)}(\mathbf{r},\mathbf{r}')$$
$$= \gamma^{(0)}(\mathbf{r},z) + C_1(\mathbf{r},z)\left(\nabla_{\mathbf{r}}k_F^2\right)\cdot\frac{\mathbf{y}}{y}$$
$$+ C_2(\mathbf{r},z)\,\nabla_{\mathbf{r}}^2k_F^2 + C_3(\mathbf{r},z)\left(\nabla_{\mathbf{r}}k_F^2\right)^2$$
$$+ C_4(\mathbf{r},z)\left[\left(\nabla_{\mathbf{r}}k_F^2\right)\cdot\frac{\mathbf{y}}{y}\right]^2$$
$$+ C_5(\mathbf{r},z)\,\nabla_{\mathbf{r}}\left[\left(\nabla_{\mathbf{r}}k_F^2\right)\cdot\frac{\mathbf{y}}{y}\right]\cdot\frac{\mathbf{y}}{y}, \tag{17}$$

where C_i are given by

$$C_1(\mathbf{r},z) = \frac{2\delta_{\sigma,\sigma'}k_F}{(2\pi)^D}\frac{\partial v(\mathbf{r},z)}{\partial z}$$
$$= -\frac{\delta_{\sigma,\sigma'}k_F^{D-3}z^2}{2(2\pi\,z)^{D/2}}J_{\frac{D}{2}-1}(z);$$

$$C_2(\mathbf{r},z) = \frac{\delta_{\sigma,\sigma'}}{(2\pi)^D}\left(v(\mathbf{r},z) + \frac{4}{3}\frac{k_F^2}{z}\frac{\partial g}{\partial z}\right)$$
$$= \frac{\delta_{\sigma,\sigma'}k_F^{D-4}z}{12(2\pi\,z)^{D/2}}\{(D-2)J_{\frac{D}{2}-1}(z) - z\,J_{\frac{D}{2}}(z)\};$$

$$C_3(\mathbf{r},z) = \frac{\delta_{\sigma,\sigma'}}{(2\pi)^D}\left(\frac{2}{3}g(\mathbf{r},z) + \frac{k_F^2}{z}\frac{\partial h(\mathbf{r},z)}{\partial z}\right)$$
$$= \frac{\delta_{\sigma,\sigma'}k_F^{D-6}}{48(2\pi\,z)^{D/2}}\{(4-D)z^2J_{\frac{D}{2}}(z)$$
$$-[(4-D)(D-2)z + z^3]J_{\frac{D}{2}-1}(z)\};$$

$$C_4(\mathbf{r},z) = \frac{k_F^2\delta_{\sigma,\sigma'}}{(2\pi)^D}\left(\frac{\partial^2h(\mathbf{r},z)}{\partial z^2} - \frac{1}{z}\frac{\partial h(\mathbf{r},z)}{\partial z}\right)$$

$$= \frac{\delta_{\sigma,\sigma'}\, k_F^{D-6} z^3}{16(2\pi\, z)^{D/2}} \{(D-2) J_{\frac{D}{2}-1}(z) - z\, J_{\frac{D}{2}}(z)\};$$

$$C_5(\mathbf{r},z) = \frac{4\delta_{\sigma,\sigma'} k_F^2}{3(2\pi)^D} \left(\frac{\partial^2 g(\mathbf{r},z)}{\partial z^2} - \frac{1}{z}\frac{\partial g(\mathbf{r},z)}{\partial z} \right)$$

$$= \frac{\delta_{\sigma,\sigma'} k_F^{D-4} z^3}{6(2\pi\, z)^{D/2}} J_{\frac{D}{2}-1}(z).$$

The D-dimensional one-particle density $n(\mathbf{r}) = \gamma(\mathbf{r},\mathbf{r})$ becomes

$$n(\mathbf{r}) = \alpha_D k_F^D \left\{ 1 + \frac{D(D-2)}{24 k_F^4} \nabla^2 k_F^2 - \frac{D(D-2)(4-D)}{96 k_F^6} (\bar{\nabla} k_F^2)^2 \right\}, \tag{18}$$

where $\alpha_D = [D\, 2^{D-2} \pi^{D/2} \Gamma(D/2)]^{-1}$. Using the density scaling relations,[15] we can invert the expression to find the local Fermi momentum as

$$k_F(\mathbf{r}) = \alpha_D^{-1/D} n^{1/D} + \frac{D-2}{24D} \alpha_D^{1/D} \frac{(\nabla n)^2}{n^{2+1/D}} + \frac{2-D}{12D} \alpha_D^{1/D} \frac{\nabla^2 n}{n^{1+1/D}}. \tag{19}$$

Both of the previous equations are consistent with earlier results.[7,10,11] Now it is straightforward to proceed with the calculation of the one-particle density matrix and the exchange energy density in 2D.

III. TWO-DIMENSIONAL CASE

A. One-particle density matrix and the kinetic energy

In the 2D case Eq. (15) simplifies to

$$I(ky) = 2\pi\, J_0(ky). \tag{20}$$

This leads to the following expression for the 2D one-particle density matrix:

$$\begin{aligned} \gamma(\mathbf{r},\mathbf{r}') &= \gamma^{(0)} + \gamma^{(2)}(\mathbf{r},\mathbf{r}') \\ &= \frac{\delta_{\sigma,\sigma'}}{\pi} \left\{ k_F^2 \frac{J_1(z)}{z} - \frac{1}{4} z J_0(z) \frac{1}{k_F} (\nabla_\mathbf{r} k_F^2) \cdot \frac{\mathbf{y}}{y} \right. \\ &\quad - \frac{1}{24} z J_1(z) \frac{\nabla_\mathbf{r}^2 k_F^2}{k_F^2} \\ &\quad + \frac{1}{12} z^2 J_0(z) \frac{1}{k_F^2} \nabla_\mathbf{r} \left((\nabla_\mathbf{r} k_F^2) \cdot \frac{\mathbf{y}}{y} \right) \cdot \frac{\mathbf{y}}{y} \\ &\quad + \frac{1}{96} z^2 J_2(z) \frac{(\nabla_\mathbf{r} k_F^2)^2}{k_F^4} \\ &\quad \left. - \frac{1}{32} z^3 J_1(z) \frac{1}{k_F^4} \left((\nabla_\mathbf{r} k_F^2) \cdot \frac{\mathbf{y}}{y} \right)^2 \right\}, \end{aligned} \tag{21}$$

This expression is the central result of this paper, and in the following it is used for further analysis.

We first notice that the one-particle density has a simple form

$$n(\mathbf{r}) = \frac{1}{2\pi} k_F^2(\mathbf{r}), \tag{22}$$

i.e., all the gradient corrections vanish in agreement with Refs. 7, 9–11, and 16. Thus, the situation is very different from the 3D case with a nonzero gradient expression.[6] Secondly, we calculate the KS kinetic energy density by inserting Eqs. (21) and (22) into Eq. (2) and find[17]

$$\begin{aligned} t_s &= -\frac{\hbar^2}{2m} \{\nabla_\mathbf{r}^2 \gamma_S(\mathbf{r},\mathbf{r}')\}_{\mathbf{r}'=\mathbf{r}} \\ &= \frac{\hbar^2 \pi}{2m} n^2(\mathbf{r}) - \frac{1}{12m} \nabla^2 n(\mathbf{r}), \end{aligned} \tag{23}$$

so that the kinetic energy becomes

$$T_s = \int d\mathbf{r}\, t_s(\mathbf{r}) = \frac{\hbar^2 \pi}{2m} \int d\mathbf{r} n^2(\mathbf{r}). \tag{24}$$

Thus we find that the gradient correction (von Weizsäcker term) to T_s is zero, in agreement with previous Kirzhnits expansion for the D-dimensional kinetic energy,[7] as well as with results obtained using alternative methods.[9–11,16,18] However, the gradient term exists for t_s. We also point out that very recently the gradient corrections for T_s have been considered at finite temperature.[19]

In their recent work, Proetto and Gross[12] have derived a rigorous condition to test the consistency of approximations made for the density and the KS kinetic energy. The condition is given by

$$\frac{\delta T_s[v_s]}{\delta v_s(\mathbf{r})} = -\int d\mathbf{r}' v_s(\mathbf{r}') \frac{\delta n[v_s](\mathbf{r}')}{\delta v_s(\mathbf{r})}, \tag{25}$$

where v_s is the KS potential. We note that the condition follows from the Euler equation minimizing the KS energy, i.e.,

$$\frac{\delta T_s}{\delta n(\mathbf{r}')} = -v_s(\mathbf{r}') + \mu, \tag{26}$$

where μ is the chemical potential. Multiplying both sides with $\delta n(\mathbf{r}')/\delta v_s(\mathbf{r})$ and integrating over $\mathbf{r}'$ directly yields Eq. (25). The condition means that $\delta T_s[n]/\delta n(\mathbf{r}') = \epsilon_F - v_s$ must be also valid. Using Eqs. (22) and (23), and $k_F = \sqrt{2m(\epsilon_F - v_s)/\hbar^2}$, we find

$$\frac{\delta T^{\mathrm{TF}}[n]}{\delta n(\mathbf{r}')} = \frac{\hbar^2}{m} \pi\, n = \frac{\hbar^2}{2m} k_F^2 = \epsilon_F - v_s. \tag{27}$$

Thus, Eq. (25) is fulfilled for the 2D (and also 3D) results of the semiclassical Kirzhnits expansion.

B. Exchange energy

Knowledge of the gradient corrections to the one-particle density matrix in Eq. (21) immediately motivates us to search for an expression for the exchange energy defined in Eq. (1). We obtain the second-order expansion of the exchange energy density in $\hbar$ in terms of the gradients of k_F:

$$\begin{aligned} e_x(\mathbf{r}) &= -\frac{1}{4} \int d^2\mathbf{r}' \frac{|\gamma(\mathbf{r},\mathbf{r}')|^2}{|\mathbf{r}-\mathbf{r}'|} \\ &= -\frac{1}{2\pi} k_F^4 \int_0^\infty dy A_1(z) \end{aligned}$$

$$- \frac{1}{24\pi}\nabla^2 k_F^2 \int_0^\infty dy A_2(z)$$
$$- \frac{1}{192\pi}\frac{(\bar{\nabla} k_F^2)^2}{k_F^2}\int_0^\infty dy A_3(z), \tag{28}$$

where

$$A_1(z) = J_1(z)^2/z^2,$$
$$A_2(z) = zJ_0(z)J_1(z) - J_1(z)^2,$$
$$A_3(z) = 3z^2 J_0(z)^2 - 2zJ_0(z)J_1(z) + (4-3z^2)J_1(z)^2$$

with $z = k_F y$. Using Green's first theorem in the integration and then the substitution $y \to z/k_F$ (see Ref. 6 for details), the expression simplifies to

$$e_x(\mathbf{r}) = -\frac{2}{3\pi^2}k_F^3 - \frac{1}{192\pi}\frac{(\nabla k_F^2)^2}{k_F^3}\int_0^\infty dz\, H(z), \tag{29}$$

where

$$H(z) \equiv 6z\, J_0(z)J_1(z) - z^2 J_0(z)^2 + (z^2-4)J_1(z)^2. \tag{30}$$

Using a regularization of divergent Coulomb integrals leads to

$$\lim_{\alpha\to 0}\int_0^\infty dz e^{-\alpha z}H(z) = \infty, \tag{31}$$

which is verified by using *Mathematica*. In other words, the exchange energy density with the standard regularization is divergent in the 2D Kirzhnits expansion. Our result agrees with the finding of Gumbs and Geldart,[13] who used perturbation theory and linear-response formalism to derive the second-order gradient terms for both the kinetic and exchange energies in D dimensions. They arrived at the same result by using the Wigner-Kirkwood expansion.[20] Hence, as confirmed in this work from the semiclassical point of view, the divergence of the systematic gradient expansion for the exchange energy seems to be an inevitable mathematical fact. However, to the best of our knowledge, the underlying *physical* reason that makes the 2D situation especially divergent, in contrast with the 1D and 3D cases, remains unknown. We hope that the present analysis encourages further examinations from that viewpoint.

The divergence of the exchange energy in 2D can be considered unfortunate in view of functional developments in 2D, although first GGAs in 2D have already been obtained,[21] and several other 2D functionals have been derived, for example, in the framework of meta GGAs.[22] A natural next step, as already discussed in Ref. 13, would be considering expansions in quasi-2DEG by introducing a finite width of the system. This would resemble the experimental situation in low-dimensional nanostructures such as in semiconductor quantum dots.

IV. SUMMARY

In summary, we have derived the second-order gradient corrections to the one-particle density matrix in the semiclassical Kirzhnits expansion in D dimensions. In two dimensions the corrections vanish in the diagonal of the density matrix, i.e., in the one-particle density. Similar vanishing occurs in the noninteracting kinetic energy and leads to the fulfillment of the consistency criterion of Ref. 12. Finally, we have shown that the exchange energy of the two-dimensional Kirzhnits expansion diverges in agreement with the linear-response theory. We hope that the present work motivates further attempts in the systematic derivation of gradient corrections in the quasi-two-dimensional electron gas.

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APPENDIX: INTERMEDIATE STEPS IN THE CALCULATION OF THE SECOND-ORDER GRADIENT CORRECTION TO THE *D*-DIMENSIONAL DENSITY MATRIX

The second-order gradient correction to the density matrix corresponds to the sum with $n = 2,3,4$ in the second term of Eq. (13). We may thus write $\gamma^{(2)}(\mathbf{r},\mathbf{r}') = B_2 + B_3 + B_4$, where

$$\begin{aligned} B_2(\mathbf{r},\mathbf{y}) &= \frac{\delta_{\sigma,\sigma'}}{(2\pi)^D}\left[\nabla_{\mathbf{r}}^2 k_F^2 v(\mathbf{r},z) + 2\left(\nabla_{\mathbf{r}} k_F^2\right)\cdot\nabla_{\mathbf{y}} v(\mathbf{r},z)\right] \\ &= \frac{\delta_{\sigma,\sigma'}}{(2\pi)^D}\left[\nabla_{\mathbf{r}}^2 k_F^2 v(\mathbf{r},z) + 2k_F\frac{\partial v}{\partial z}\left(\nabla_{\mathbf{r}} k_F^2\right)\cdot\frac{\mathbf{y}}{y}\right] \\ &= \frac{-k_F^{D-4}}{4(2\pi)^{\frac{D}{2}} z^{\frac{D-2}{2}}}\left\{2k_F z J_{\frac{D}{2}-1}(z)\left(\nabla_{\mathbf{r}} k_F^2\right)\cdot\frac{\mathbf{y}}{y}\right. \\ &\quad \left. + \left[zJ_{\frac{D}{2}}(z) - (D-2)J_{\frac{D}{2}-1}(z)\right]\nabla_{\mathbf{r}}^2 k_F^2\right\}, \end{aligned} \tag{A1}$$

$$\begin{aligned} B_3(\mathbf{r},\mathbf{y}) &= \frac{2\delta_{\sigma,\sigma'}}{3(2\pi)^D}\left\{2\nabla_{\mathbf{r}}^2 k_F^2 \frac{k_F^2}{z}\frac{\partial g}{\partial z} + \left(\nabla_{\mathbf{r}} k_F^2\right)^2 g(\mathbf{r},z)\right. \\ &\quad \left. + 2k_F^2 \nabla_{\mathbf{r}}\left[\left(\nabla_{\mathbf{r}} k_F^2\right)\cdot\frac{\mathbf{y}}{y}\right]\cdot\frac{\mathbf{y}}{y}\left(\frac{\partial^2 g}{\partial z^2} - \frac{1}{z}\frac{\partial g}{\partial z}\right)\right\} \\ &= \frac{-k_F^{D-6}}{12(2\pi)^{\frac{D}{2}} z^{\frac{D-2}{2}}}\left\{\left[2(D-2)k_F^2 J_{\frac{D}{2}-1}(z)\right.\right. \\ &\quad \left. - 2k_F^2 z J_{\frac{D}{2}}(z)\right]\nabla_{\mathbf{r}}^2 k_F^2 \\ &\quad - 2k_F^2 z^2 J_{\frac{D}{2}-1}(z)\nabla_{\mathbf{r}}\left[\left(\nabla_{\mathbf{r}} k_F^2\right)\cdot\frac{\mathbf{y}}{y}\right]\cdot\frac{\mathbf{y}}{y} \\ &\quad + [((4-D)(D-2)+z^2)J_{\frac{D}{2}-1}(z) \\ &\quad \left. - (4-D)zJ_{\frac{D}{2}}(z)]\left(\nabla_{\mathbf{r}} k_F^2\right)^2\right\}, \end{aligned} \tag{A2}$$

$$\begin{aligned} B_4(\mathbf{r},\mathbf{y}) &= \frac{\delta_{\sigma,\sigma'}}{(2\pi)^D}\left\{\left(\nabla_{\mathbf{r}} k_F^2\right)^2 \frac{k_F^2}{z}\frac{\partial h}{\partial z}\right. \\ &\quad \left. + k_F^2\left[\left(\nabla_{\mathbf{r}} k_F^2\right)\cdot\frac{\mathbf{y}}{y}\right]^2\left(\frac{\partial^2 h}{\partial z^2} - \frac{1}{z}\frac{\partial h}{\partial z}\right)\right\} \\ &= \frac{k_F^{D-6}}{16(2\pi)^{\frac{D}{2}} z^{\frac{D-2}{2}}}\left\{\left[(D-2)z^2 J_{\frac{D}{2}-1}(z)\right.\right. \end{aligned}$$

$$
-z^3 J_{\frac{D}{2}}(z)\Big]\left[\left(\nabla_{\mathbf{r}} k_F^2\right)\cdot\frac{\mathbf{y}}{y}\right]^2
+\Big[((4-D)(D-2)+z^2)J_{\frac{D}{2}-1}(z)
-(4-D)zJ_{\frac{D}{2}}(z)\Big]\left(\nabla_{\mathbf{r}} k_F^2\right)^2\Big\}, \qquad \text{(A3)}
$$

with expressions

$$
\begin{aligned}
v(\mathbf{r},z) &= \int d^D\mathbf{k}\,\delta'\left[E_F-\frac{1}{2}k^2\right]e^{i\mathbf{k}\cdot\mathbf{y}}\\
&= \frac{k_F^{D-4}}{4}[(d-2)I(z)+zI'(z)]\\
&= \frac{(2\pi)^{\frac{D}{2}}k_F^{D-4}}{4z^{\frac{D-2}{2}}}\{(D-2)J_{\frac{D}{2}-1}(z)-zJ_{\frac{D}{2}}(z)\}, \qquad \text{(A4)}
\end{aligned}
$$

$$
\begin{aligned}
g(\mathbf{r},z) &= \int d^D\mathbf{k}\,\delta''\left[E_F-\frac{1}{2}k^2\right]e^{i\mathbf{k}\cdot\mathbf{y}}\\
&= \frac{k_F^{D-6}}{8}\{[D^2-6D+8]I(z)+(2D-5)zI'(z)\\
&\quad +z^2I''(z)\}\\
&= \frac{(2\pi)^{\frac{D}{2}}k_F^{D-6}}{8z^{\frac{D-2}{2}}}\{(4-D)zJ_{\frac{D}{2}}(z)\\
&\quad -[(4-D)(D-2)+z^2]J_{\frac{D}{2}-1}(z)\}, \qquad \text{(A5)}
\end{aligned}
$$

$$
\begin{aligned}
h(\mathbf{r},z) &= \int d^D\mathbf{k}\,\delta'''\left[E_F-\frac{1}{2}k^2\right]e^{i\mathbf{k}\cdot\mathbf{y}}\\
&= \frac{k_F^{D-8}}{16}\{[D^3-12D^2+44D-48]I(z)\\
&\quad +3(D^2-7D+11)zI'(z)+3(D-3)z^2I''(z)\\
&\quad +z^3I^{(3)}(z)\}\\
&= \frac{(2\pi)^{\frac{D}{2}}k_F^{D-8}}{16z^{\frac{D-2}{2}}}\{(4-D)[(6-D)(D-2)\\
&\quad +2z^2]J_{\frac{D}{2}-1}(z)\\
&\quad -z[(6-D)(4-D)-z^2]J_{\frac{D}{2}}(z)\}. \qquad \text{(A6)}
\end{aligned}
$$

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