

Inhomogeneity corrections to the ground-state properties of itinerant ferromagnets*

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A first-principles potential for an itinerant spin-polarized electron gas has allowed a more fundamental study of ground-state properties in itinerant ferromagnets. The contribution of additional terms accounting for the highly inhomogeneous spin-density profile, found in most ferromagnetic materials, is presented. These are evaluated rigorously in the high-density limit, and results are given for arbitrary ratios of spin-up and spin-down densities. Forms are also derived for extending the results to lower spin densities.

I. INTRODUCTION

The numerical sophistication for calculating ground-state properties of solids has been increasing rapidly. In the last decade more and more accurate self-consistent techniques have been developed, reaching the point where the fundamental question of the importance of electron-electron interactions can now be tested.¹

Initial studies were naturally confined to simple metals. Recently, however, greater effort has been made toward a first-principles understanding of complex metals; in particular the transition series.

Such systems, being itinerant ferromagnets, have an unequal density of spin-up and spin-down electrons. Thus, a first-principles exchange and correlation potential must depend on both spin densities.

The first to calculate a form for the spin-polarized exchange and correlation potential were von Barth and Hedin² (vBH). Assuming slowly varying spin densities $\rho_\uparrow(\vec{r})$ and $\rho_\downarrow(\vec{r})$ their exchange and correlation energy E^{xc} was approximated by a local form $E_{\vec{r}}^{xc}$, i.e.,

$$E^{xc}(\rho_\uparrow(\vec{r}), \rho_\downarrow(\vec{r})) \approx E_{\vec{r}}^{xc} \\ \equiv \int d\vec{r} (\rho_\uparrow(\vec{r}) + \rho_\downarrow(\vec{r})) \\ \times \epsilon_{xc}(\rho_\uparrow(\vec{r}), \rho_\downarrow(\vec{r})) . \quad (1)$$

In Equation (1), ϵ_{xc} is the exchange and correlation energy per particle of a spin-polarized interacting electron gas.

Wang and Callaway³ have applied this potential to various properties of nickel and iron. Their detailed study shows that the vBH potential produces significant improvement over the non-spin-polarized potential. Nevertheless, sizable discrepancies between theory and experiment do remain³ raising the possibility that nonlocal contributions to Eq. (1) are

important.

The purpose of this work is to present such corrections to Eq. (1) with the hope of resolving some of these fundamental questions.

In Sec. II we give a brief formulation and *rigorous* results valid in the high-density limit (HDL). In Sec. III we derive forms which are indispensable for a fundamental extension of these results to metallic densities.

II. FORMULATION AND RESULTS IN THE HDL

The additional nonlocal contributions we wish to consider here are

$$E_{nl}^{xc} \approx \int d\vec{r} [B_{\uparrow\uparrow}^{xc}(\rho_\uparrow(\vec{r}), \rho_\downarrow(\vec{r})) |\nabla \rho_\uparrow(\vec{r})|^2 \\ + B_{\uparrow\downarrow}^{xc}(\rho_\uparrow(\vec{r}), \rho_\downarrow(\vec{r})) |\nabla \rho_\downarrow(\vec{r})|^2 \\ + B_{\downarrow\downarrow}^{xc}(\rho_\uparrow(\vec{r}), \rho_\downarrow(\vec{r})) \nabla \rho_\uparrow(\vec{r}) \cdot \nabla \rho_\downarrow(\vec{r})] \quad (2)$$

and $E^{xc} = E_{\uparrow\uparrow}^{xc} + E_{nl}^{xc}$. To determine the coefficients B^{xc} consider two weak external fields $V_\uparrow(\vec{k})$ and $V_\downarrow(\vec{k})$ (of Fourier component \vec{k}) applied to an interacting uniform electron gas of arbitrary spin densities ρ_\uparrow and ρ_\downarrow . Allow $V_\uparrow(\vec{k})$ to couple only to the spin up and $V_\downarrow(\vec{k})$ to spin down. In other words, the perturbation H_I is given by

$$H_I = V_\uparrow(\vec{k}) \hat{\rho}_\uparrow(\vec{k}) + V_\downarrow(\vec{k}) \hat{\rho}_\downarrow(\vec{k}) , \quad (3)$$

where $\hat{\rho}_\uparrow(\vec{k})$ and $\hat{\rho}_\downarrow(\vec{k})$ are the spin-density up and down operators, respectively.

The analysis now proceeds in identical fashion to that presented by Rasolt and Geldart⁴ (RG) for the two-component electron-hole liquid. The only difference being the sign of the interactions. We write below only the final results.

First to second order in H_I ,

$$\begin{aligned} \Delta E^{xc}(\bar{k}) + \Delta T_s(\bar{k}) &= \frac{1}{2} [(\rho_1(\bar{k}))^2 \chi_{11}(\bar{k}) \\ &\quad + (\rho_1(\bar{k}))^2 \chi_{1\bar{1}}(\bar{k}) \\ &\quad - 2\rho_1(\bar{k})\rho_{\bar{1}}(\bar{k})\chi_{1\bar{1}}(\bar{k})] \\ &\quad \times [\chi_{11}(\bar{k})\chi_{1\bar{1}}(\bar{k}) - (\chi_{11}(\bar{k}))^2]^{-1} \\ &\quad - (2\pi e^2/\bar{k}^2)(\rho_1(\bar{k}) + \rho_{\bar{1}}(\bar{k}))^2 \end{aligned} \quad (4)$$

Here the χ 's are the reducible spin-spin response functions. In terms of the irreducible response functions $\pi(\bar{k})$, the $\chi(\bar{k})$ are given by

$$\chi_{11}(\bar{k}) = \frac{\pi_{11}(\bar{k}) + (4\pi e^2/\bar{k}^2)\Delta(\bar{k})}{\epsilon(\bar{k})}, \quad (5)$$

$$\chi_{1\bar{1}}(\bar{k}) = \frac{\pi_{1\bar{1}}(\bar{k}) + (4\pi e^2/\bar{k}^2)\Delta(\bar{k})}{\epsilon(\bar{k})}, \quad (6)$$

$$\chi_{\bar{1}\bar{1}}(\bar{k}) = \frac{\pi_{\bar{1}\bar{1}}(\bar{k}) + (4\pi e^2/\bar{k}^2)\Delta(\bar{k})}{\epsilon(\bar{k})}, \quad (7)$$

$$\Delta(\bar{k}) = \pi_{11}(\bar{k})\pi_{1\bar{1}}(\bar{k}) - (\pi_{11}(\bar{k}))^2, \quad (8)$$

$$\begin{aligned} \epsilon(\bar{k}) &= 1 + (4\pi e^2/\bar{k}^2)[\pi_{11}(\bar{k}) + \pi_{1\bar{1}}(\bar{k}) \\ &\quad + 2\pi_{1\bar{1}}(\bar{k})], \end{aligned} \quad (9)$$

and $\Delta T_s(\bar{k})$ is the kinetic energy of the noninteracting electron gas to second order in H_I , i.e.,

$$\Delta T_s(\bar{k}) = -\frac{1}{2} \frac{(\rho_1(\bar{k}))^2}{\pi_{11}^0(\bar{k})} - \frac{\rho_{\bar{1}}((\bar{k}))^2}{\pi_{1\bar{1}}^0(\bar{k})}, \quad (10)$$

where $\pi_{11}^0(\bar{k})$ and $\pi_{1\bar{1}}^0(\bar{k})$ are the Lindhard function (for a single spin) for spin up and spin down, respectively.

Using Eqs. (2)–(10), we get the desired relations between B^{xc} and the irreducible spin functions $\pi(\bar{k})$ given by the coefficients of the \bar{k}^2 term in the expansion of the following functions:

$$\frac{1}{2} \left[-\frac{\pi_{11}(\bar{k})}{\Delta(\bar{k})} + \frac{1}{\pi_{11}^0(\bar{k})} \right] = \text{const} + B_{11}^{xc} \bar{k}^2, \quad (11)$$

$$\frac{1}{2} \left[-\frac{\pi_{1\bar{1}}(\bar{k})}{\Delta(\bar{k})} + \frac{1}{\pi_{1\bar{1}}^0(\bar{k})} \right] = \text{const} + B_{1\bar{1}}^{xc} \bar{k}^2, \quad (12)$$

$$\frac{\pi_{1\bar{1}}(\bar{k})}{\Delta(\bar{k})} = \text{const} + B_{1\bar{1}}^{xc} \bar{k}^2. \quad (13)$$

From Eqs. (11)–(13), we see that to evaluate B^{xc} all we need is the expansion of the $\pi(\bar{k})$ to order \bar{k}^2 , i.e.,

$$\pi_{11}(\bar{k}) \approx a_{11}^{-1} + b_{11} \bar{k}^2,$$

$$\pi_{1\bar{1}}(\bar{k}) \approx a_{1\bar{1}}^{-1} + b_{1\bar{1}} \bar{k}^2,$$

$$\pi_{\bar{1}\bar{1}}(\bar{k}) \approx a_{\bar{1}\bar{1}}^{-1} + b_{\bar{1}\bar{1}} \bar{k}^2.$$

The difficulty of evaluating B^{xc} clearly resides in calculating the b coefficients. We restrict our calculation here to the HDL, in which case identical to RG we see that Eqs. (11)–(13) simplify to

$$\frac{1}{2} \left[-\frac{1}{\pi_{11}(\bar{k})} + \frac{1}{\pi_{11}^0(\bar{k})} \right] = \text{const} + B_{11}^{xc} \bar{k}^2,$$

$$\frac{1}{2} \left[-\frac{1}{\pi_{1\bar{1}}(\bar{k})} + \frac{1}{\pi_{1\bar{1}}^0(\bar{k})} \right] = \text{const} + B_{1\bar{1}}^{xc} \bar{k}^2,$$

$$\frac{\pi_{1\bar{1}}(\bar{k})}{\pi_{11}(\bar{k})\pi_{1\bar{1}}(\bar{k})} = \text{const} + B_{1\bar{1}}^{xc} \bar{k}^2.$$

From the above relations, it is evident that the analysis required to evaluate the b 's follows closely that given in RG. For the sake of brevity, we will not repeat this lengthy analysis, but simply write down the final results for B^{xc} .

The reader interested in finer details will note that subtle differences do arise from the screened interaction [Fig. 4(c) of RG] having only a single spin per bubble diagram.

Defining the dimensionless quantities C^{xc} as

$$B_{11}^{xc} \equiv \frac{e^2 C_{11}^{xc}}{\rho_1^{4/3}}, \quad B_{1\bar{1}}^{xc} \equiv \frac{e^2 C_{1\bar{1}}^{xc}}{\rho_{\bar{1}}^{4/3}}, \quad (14)$$

$$B_{1\bar{1}}^{xc} \equiv \frac{e^2 C_{1\bar{1}}^{xc}}{(\rho_1 \rho_{\bar{1}})^{2/3}},$$

we get

$$C_{11}^{xc} = [1/(6\pi^2)^{4/3}] (Z_{11}^C - \frac{7}{72} \pi),$$

$$C_{1\bar{1}}^{xc} = [1/(6\pi^2)^{4/3}] (Z_{1\bar{1}}^C - \frac{7}{72} \pi), \quad (15)$$

$$C_{1\bar{1}}^{xc} = [2/(6\pi^2)^{4/3}] Z_{1\bar{1}}^C,$$

where

$$\begin{aligned} Z_{11}^C &= \int_0^\infty dy \left\{ \frac{1}{36} \left[1 - \frac{H(\beta, y)}{G(\beta, y)} \right] \left[\frac{9y^2 + 13y^2}{(y^2 + 1)^3} \right] + \frac{1}{4} \ln[G(\beta, y)] \left[\frac{y^2(3 - y^2)}{(y^2 + 1)^3} \right] \right. \\ &\quad \left. - \frac{1}{12} \frac{1}{(y^2 + 1)^2} \frac{1}{G(\beta, y)} \left[-1 + \frac{1}{2} \frac{I(\beta, y)}{G(\beta, y)} + \frac{1}{6} \left(\frac{I(\beta, y)}{G(\beta, y)} \right)^2 - \frac{1}{2} \frac{J(\beta, y)}{G(\beta, y)} \right] \right\}, \end{aligned} \quad (16)$$

$$Z_{11}^c = \int_0^\infty dy \left\{ \frac{1}{72} \beta \frac{H(\beta, y)}{G(\beta, y)} \left(\frac{9y^4 + 13y^2}{(y^2 + 1)^3} \right) + \frac{1}{72} \frac{1}{\beta} \frac{H(1/\beta, y)}{G(1/\beta, y)} \left(\frac{9y^4 + 13y^2}{(y^2 + 1)^3} \right) \right. \\ \left. - \frac{1}{12} \frac{1}{\beta^2} \frac{1}{(y^2 + 1/\beta^2)} \frac{1}{(y^2 + 1)} \frac{1}{G(\beta, y)} \left[-1 + \frac{1}{2} \frac{I(\beta, y)}{G(\beta, y)} + \frac{1}{6} \left(\frac{I(\beta, y)}{G(\beta, y)} \right)^2 - \frac{1}{2} \frac{J(\beta, y)}{G(\beta, y)} \right] \right\}, \quad (17)$$

and Z_{11}^c is identical to Z_{11}^c with $\beta \rightarrow 1/\beta$. In Eqs. (16) and (17),

$$G(\beta, y) = R(y) + 1/\beta - y \tan^{-1}(1/\beta y), \quad (18)$$

$$R(y) = 1 - y \tan^{-1}(1/y), \quad (19)$$

$$H(\beta, y) = (1/\beta^3)(y^2 + 1/\beta^2)^{-1}, \quad (20)$$

$$I(\beta, y) = -(1 + y^2)^{-1} - H(\beta, y), \quad (21)$$

and

$$J(\beta, y) = -(1 + y^2)^{-2} - \beta [H(\beta, y)]^2, \quad (22)$$

with $\beta \equiv (\rho_1/\rho_1)^{1/3}$.

Equations (14)–(22) have been evaluated for a range of spin-up to spin-down density ratios β , and the results are displayed in Fig. 1. The most striking feature of these results is the strong and different dependence of each of the C^{xc} on β . No single component calculation is adequate for predicting this wide range of variation.

The above calculation is formally valid in the HDL. It can be argued that ferromagnetism does not even exist in the HDL, hence what use are these results? First, single component studies strongly suggest that the variation of C^{xc} away from the HDL should be weak. Hence application of the above results should give a good indication of the importance and trends of E_{nl}^{xc} . Secondly, any approximate scheme for extending the above results to metallic densities can now be tested against the rigorous results in the HDL.

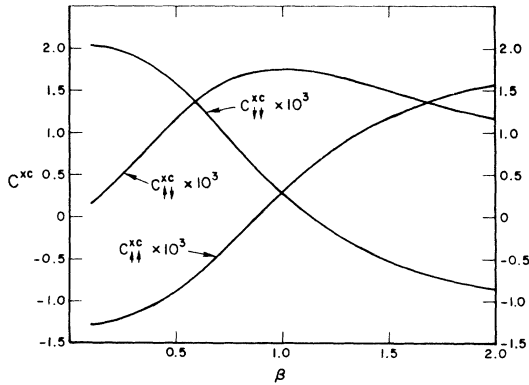


FIG. 1. Calculated HDL contributions to the exchange and correlation gradient coefficients (see Sec. II) for spin-polarized electron gas as a function of spin-up to spin-down densities $\beta \equiv (\rho_1/\rho_1)^{1/3}$.

Clearly the extension to the metallic range is important. In Sec. III we derive *exact simplified* relations for $b\bar{k}^2$ with the intent that these will make such a fundamental extension possible.

III. GENERAL FORMS FOR b_{1i} , b_{11} , AND b_{11}

In this section, we derive expressions for b_{1i} , b_{11} , and b_{11} which are exact to all order in e^2 . Clearly a straightforward substitution in Eqs. (11)–(13) then yields B^{xc} for the full range of spin-up and spin-down densities.

We proceed from the *reducible* scattering functions $\Gamma_{11}(\bar{k})$, $\Gamma_{11}(\bar{k})$, and $\Gamma_{11}(\bar{k})$.⁵ Their graphical representation in terms of the *irreducible*⁵ scattering functions $\gamma_{11}(\bar{k})$, $\gamma_{11}(\bar{k})$, and $\gamma_{11}(\bar{k})$ are displayed in Fig. 2. Their relation to the desired screening functions $\pi_{11}(\bar{k})$, $\pi_{11}(\bar{k})$, and $\pi_{11}(\bar{k})$ are shown in Fig. 3.

In the usual matrix notation⁵ the following set of equations for $\Gamma(\bar{k})$ represent Fig. 2:

$$\Gamma_{11}(\bar{k}) = \gamma_{11}(\bar{k}) + \gamma_{11}(\bar{k})P_{11}(\bar{k})\Gamma_{11}(\bar{k}) \\ + \gamma_{11}(\bar{k})P_{11}(\bar{k})\Gamma_{11}(\bar{k}), \quad (23)$$

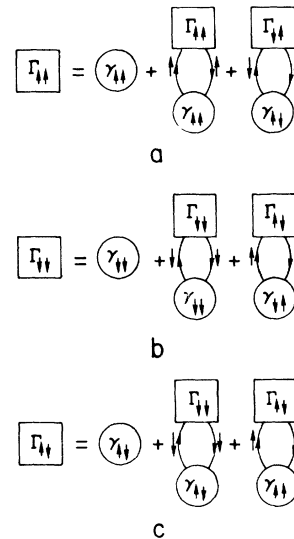


FIG. 2. Graphical representation for the reducible scattering functions Γ_{11} , Γ_{11} , and Γ_{11} in terms of the irreducible scattering functions γ_{11} , γ_{11} , and γ_{11} .

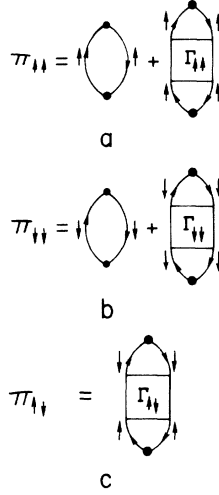


FIG. 3. Graphical representation for the irreducible screening functions $\pi_{\uparrow\uparrow}$, $\pi_{\uparrow\downarrow}$, and $\pi_{\downarrow\downarrow}$ in terms of $\Gamma_{\uparrow\uparrow}$, $\Gamma_{\uparrow\downarrow}$, and $\Gamma_{\downarrow\downarrow}$.

$$\Gamma_{\uparrow\uparrow}(\bar{\mathbf{k}}) = \gamma_{\uparrow\uparrow}(\bar{\mathbf{k}}) + \Gamma_{\uparrow\uparrow}(\bar{\mathbf{k}})P_{\uparrow\uparrow}(\bar{\mathbf{k}})\gamma_{\uparrow\uparrow}(\bar{\mathbf{k}}) + \Gamma_{\uparrow\downarrow}(\bar{\mathbf{k}})P_{\uparrow\downarrow}(\bar{\mathbf{k}})\gamma_{\uparrow\downarrow}(\bar{\mathbf{k}}) , \quad (24)$$

$$\Gamma_{\uparrow\downarrow}(\bar{\mathbf{k}}) = \gamma_{\uparrow\downarrow}(\bar{\mathbf{k}}) + \gamma_{\uparrow\downarrow}(\bar{\mathbf{k}})P_{\uparrow\downarrow}(\bar{\mathbf{k}})\Gamma_{\uparrow\downarrow}(\bar{\mathbf{k}}) + \gamma_{\downarrow\downarrow}(\bar{\mathbf{k}})P_{\downarrow\downarrow}(\bar{\mathbf{k}})\Gamma_{\downarrow\downarrow}(\bar{\mathbf{k}}) , \quad (25)$$

$$\Gamma_{\downarrow\downarrow}(\bar{\mathbf{k}}) = \gamma_{\downarrow\downarrow}(\bar{\mathbf{k}}) + \Gamma_{\downarrow\downarrow}(\bar{\mathbf{k}})P_{\downarrow\downarrow}(\bar{\mathbf{k}})\gamma_{\downarrow\downarrow}(\bar{\mathbf{k}}) + \Gamma_{\uparrow\downarrow}(\bar{\mathbf{k}})P_{\uparrow\downarrow}(\bar{\mathbf{k}})\gamma_{\uparrow\downarrow}(\bar{\mathbf{k}}) , \quad (26)$$

$$\Gamma_{\uparrow\uparrow}(\bar{\mathbf{k}}) = \gamma_{\uparrow\uparrow}(\bar{\mathbf{k}}) + \gamma_{\uparrow\uparrow}(\bar{\mathbf{k}})P_{\uparrow\uparrow}(\bar{\mathbf{k}})\Gamma_{\uparrow\uparrow}(\bar{\mathbf{k}}) + \gamma_{\uparrow\downarrow}(\bar{\mathbf{k}})P_{\uparrow\downarrow}(\bar{\mathbf{k}})\Gamma_{\uparrow\downarrow}(\bar{\mathbf{k}}) , \quad (27)$$

$$\Gamma_{\uparrow\downarrow}(\bar{\mathbf{k}}) = \gamma_{\uparrow\downarrow}(\bar{\mathbf{k}}) + \Gamma_{\uparrow\downarrow}(\bar{\mathbf{k}})P_{\uparrow\downarrow}(\bar{\mathbf{k}})\gamma_{\uparrow\downarrow}(\bar{\mathbf{k}}) + \Gamma_{\downarrow\downarrow}(\bar{\mathbf{k}})P_{\downarrow\downarrow}(\bar{\mathbf{k}})\gamma_{\downarrow\downarrow}(\bar{\mathbf{k}}) , \quad (28)$$

$$\Gamma_{\downarrow\downarrow}(\bar{\mathbf{k}}) = \gamma_{\downarrow\downarrow}(\bar{\mathbf{k}}) + \gamma_{\downarrow\downarrow}(\bar{\mathbf{k}})P_{\downarrow\downarrow}(\bar{\mathbf{k}})\Gamma_{\downarrow\downarrow}(\bar{\mathbf{k}}) + \gamma_{\uparrow\downarrow}(\bar{\mathbf{k}})P_{\uparrow\downarrow}(\bar{\mathbf{k}})\Gamma_{\uparrow\downarrow}(\bar{\mathbf{k}}) , \quad (29)$$

and

$$\Gamma_{\uparrow\downarrow}(\bar{\mathbf{k}}) = \gamma_{\uparrow\downarrow}(\bar{\mathbf{k}}) + \Gamma_{\uparrow\downarrow}(\bar{\mathbf{k}})P_{\uparrow\downarrow}(\bar{\mathbf{k}})\gamma_{\uparrow\downarrow}(\bar{\mathbf{k}}) + \Gamma_{\downarrow\downarrow}(\bar{\mathbf{k}})P_{\downarrow\downarrow}(\bar{\mathbf{k}})\gamma_{\downarrow\downarrow}(\bar{\mathbf{k}}) , \quad (30)$$

where $P_{\uparrow\uparrow}(\bar{\mathbf{k}})$ and $P_{\downarrow\downarrow}(\bar{\mathbf{k}})$ are given by

$$P_{\uparrow\uparrow}(\bar{\mathbf{k}}) \equiv R_{\uparrow\uparrow}(\bar{\mathbf{k}})\delta_{p,p'} = S_{\uparrow}(p + \frac{1}{2}\bar{\mathbf{k}})S_{\uparrow}(p - \frac{1}{2}\bar{\mathbf{k}})\delta_{p,p'} , \quad (31)$$

and

$$P_{\downarrow\downarrow}(\bar{\mathbf{k}}) \equiv R_{\downarrow\downarrow}(\bar{\mathbf{k}})\delta_{p,p'} = S_{\downarrow}(p + \frac{1}{2}\bar{\mathbf{k}})S_{\downarrow}(p - \frac{1}{2}\bar{\mathbf{k}})\delta_{p,p'} , \quad (32)$$

with $p \equiv (\bar{p}, p_0)$ and $S_{\uparrow}, S_{\downarrow}$ are the *full* single-particle propagators for spin up and down, respectively.

Some matrix algebra using Eqs. (23)–(32) yields the following relations:

$$\begin{aligned} \Gamma_{\uparrow\uparrow}(\bar{\mathbf{k}}) - \Gamma_{\uparrow\uparrow}(0) &= \Gamma_{\uparrow\uparrow}(0)[P_{\uparrow\uparrow}(\bar{\mathbf{k}}) - P_{\uparrow\uparrow}(0)]\Gamma_{\uparrow\uparrow}(\bar{\mathbf{k}}) + \Gamma_{\uparrow\uparrow}(0)[P_{\uparrow\downarrow}(\bar{\mathbf{k}}) - P_{\uparrow\downarrow}(0)]\Gamma_{\uparrow\downarrow}(\bar{\mathbf{k}}) \\ &\quad + [\Gamma_{\uparrow\downarrow}(0)P_{\uparrow\downarrow}(0)\delta\gamma_{\uparrow\downarrow}(\bar{\mathbf{k}}) + (1 + \Gamma_{\uparrow\downarrow}(0)P_{\uparrow\downarrow}(0))\delta\gamma_{\uparrow\downarrow}(\bar{\mathbf{k}})][1 + P_{\uparrow\uparrow}(\bar{\mathbf{k}})\Gamma_{\uparrow\uparrow}(\bar{\mathbf{k}})] \\ &\quad + [\Gamma_{\uparrow\downarrow}(0)P_{\uparrow\downarrow}(0)\delta\gamma_{\uparrow\downarrow}(\bar{\mathbf{k}}) + (1 + \Gamma_{\uparrow\downarrow}(0)P_{\uparrow\downarrow}(0))\delta\gamma_{\uparrow\downarrow}(\bar{\mathbf{k}})]P_{\uparrow\downarrow}(\bar{\mathbf{k}})\Gamma_{\uparrow\downarrow}(\bar{\mathbf{k}}) , \end{aligned} \quad (33)$$

$$\begin{aligned} \Gamma_{\uparrow\downarrow}(\bar{\mathbf{k}}) - \Gamma_{\uparrow\downarrow}(0) &= \Gamma_{\uparrow\downarrow}(0)[P_{\uparrow\downarrow}(\bar{\mathbf{k}}) - P_{\uparrow\downarrow}(0)]\Gamma_{\uparrow\downarrow}(\bar{\mathbf{k}}) + \Gamma_{\uparrow\downarrow}(0)[P_{\downarrow\downarrow}(\bar{\mathbf{k}}) - P_{\downarrow\downarrow}(0)]\Gamma_{\downarrow\downarrow}(\bar{\mathbf{k}}) \\ &\quad + [\Gamma_{\uparrow\downarrow}(0)P_{\uparrow\downarrow}(0)\delta\gamma_{\uparrow\downarrow}(\bar{\mathbf{k}}) + (1 + \Gamma_{\uparrow\downarrow}(0)P_{\uparrow\downarrow}(0))\delta\gamma_{\uparrow\downarrow}(\bar{\mathbf{k}})][1 + P_{\uparrow\uparrow}(\bar{\mathbf{k}})\Gamma_{\uparrow\uparrow}(\bar{\mathbf{k}})] \\ &\quad + [\Gamma_{\uparrow\downarrow}(0)P_{\uparrow\downarrow}(0)\delta\gamma_{\uparrow\downarrow}(\bar{\mathbf{k}}) + (1 + \Gamma_{\uparrow\downarrow}(0)P_{\uparrow\downarrow}(0))\delta\gamma_{\uparrow\downarrow}(\bar{\mathbf{k}})]P_{\uparrow\downarrow}(\bar{\mathbf{k}})\Gamma_{\uparrow\downarrow}(\bar{\mathbf{k}}) , \end{aligned} \quad (34)$$

and

$$\begin{aligned} \Gamma_{\downarrow\downarrow}(\bar{\mathbf{k}}) - \Gamma_{\downarrow\downarrow}(0) &= \Gamma_{\downarrow\downarrow}(0)[P_{\downarrow\downarrow}(\bar{\mathbf{k}}) - P_{\downarrow\downarrow}(0)]\Gamma_{\downarrow\downarrow}(\bar{\mathbf{k}}) + \Gamma_{\downarrow\downarrow}(0)[P_{\uparrow\downarrow}(\bar{\mathbf{k}}) - P_{\uparrow\downarrow}(0)]\Gamma_{\uparrow\downarrow}(\bar{\mathbf{k}}) \\ &\quad + [\Gamma_{\uparrow\downarrow}(0)P_{\uparrow\downarrow}(0)\delta\gamma_{\uparrow\downarrow}(\bar{\mathbf{k}}) + (1 + \Gamma_{\uparrow\downarrow}(0)P_{\uparrow\downarrow}(0))\delta\gamma_{\uparrow\downarrow}(\bar{\mathbf{k}})][1 + P_{\uparrow\uparrow}(\bar{\mathbf{k}})\Gamma_{\uparrow\uparrow}(\bar{\mathbf{k}})] \\ &\quad + [\Gamma_{\uparrow\downarrow}(0)P_{\uparrow\downarrow}(0)\gamma_{\uparrow\downarrow}(\bar{\mathbf{k}}) + (1 + \Gamma_{\uparrow\downarrow}(0)P_{\uparrow\downarrow}(0))\delta\gamma_{\uparrow\downarrow}(\bar{\mathbf{k}})]P_{\uparrow\downarrow}(\bar{\mathbf{k}})\Gamma_{\uparrow\downarrow}(\bar{\mathbf{k}}) , \end{aligned} \quad (35)$$

where $\delta\gamma(\bar{\mathbf{k}}) \equiv \gamma(\bar{\mathbf{k}}) - \gamma(0)$. Now define the following vertex functions:

$$\Lambda_{\uparrow\uparrow}(\bar{\mathbf{k}}) = \lambda + \Gamma_{\uparrow\uparrow}(\bar{\mathbf{k}})P_{\uparrow\uparrow}(\bar{\mathbf{k}})\lambda , \quad (36)$$

$$\Lambda_{\uparrow\downarrow}(\bar{\mathbf{k}}) = \lambda + \Gamma_{\uparrow\downarrow}(\bar{\mathbf{k}})P_{\uparrow\downarrow}(\bar{\mathbf{k}})\lambda , \quad (37)$$

and

$$\Lambda_{\downarrow\downarrow}(\bar{\mathbf{k}}) = \Gamma_{\downarrow\downarrow}(\bar{\mathbf{k}})P_{\downarrow\downarrow}(\bar{\mathbf{k}})\lambda , \quad (38)$$

where λ is a column vector with components $\lambda_p = 1$. Some additional matrix algebra then yields

$$\begin{aligned} \pi_{\uparrow\uparrow}(\bar{\mathbf{k}}) - \pi_{\uparrow\uparrow}(0) &= \tilde{\Lambda}_{\uparrow\uparrow}(0)[P_{\uparrow\uparrow}(\bar{\mathbf{k}}) - P_{\uparrow\uparrow}(0)]\Lambda_{\uparrow\uparrow}(\bar{\mathbf{k}}) + \tilde{\Lambda}_{\uparrow\uparrow}(0)[P_{\uparrow\uparrow}(\bar{\mathbf{k}}) - P_{\uparrow\uparrow}(0)]\Lambda_{\uparrow\uparrow}(\bar{\mathbf{k}}) \\ &\quad + [\tilde{\Lambda}_{\uparrow\uparrow}(0)P_{\uparrow\uparrow}(0)\delta\gamma_{\uparrow\uparrow}(\bar{\mathbf{k}}) + \tilde{\Lambda}_{\uparrow\uparrow}(0)P_{\uparrow\uparrow}(0)\delta\gamma_{\uparrow\uparrow}(\bar{\mathbf{k}})]P_{\uparrow\uparrow}(\bar{\mathbf{k}})\Lambda_{\uparrow\uparrow}(\bar{\mathbf{k}}) \\ &\quad + [\tilde{\Lambda}_{\uparrow\uparrow}(0)P_{\uparrow\uparrow}(0)\delta\gamma_{\uparrow\uparrow}(\bar{\mathbf{k}}) + \tilde{\Lambda}_{\uparrow\uparrow}(0)P_{\uparrow\uparrow}(0)\delta\gamma_{\uparrow\uparrow}(\bar{\mathbf{k}})]P_{\uparrow\uparrow}(\bar{\mathbf{k}})\Lambda_{\uparrow\uparrow}(\bar{\mathbf{k}}) , \end{aligned} \quad (39)$$

$$\begin{aligned} \pi_{\uparrow\downarrow}(\bar{\mathbf{k}}) - \pi_{\uparrow\downarrow}(0) &= \tilde{\Lambda}_{\uparrow\downarrow}(0)[P_{\uparrow\downarrow}(\bar{\mathbf{k}}) - P_{\uparrow\downarrow}(0)]\Lambda_{\uparrow\downarrow}(\bar{\mathbf{k}}) + \tilde{\Lambda}_{\uparrow\downarrow}(0)[P_{\uparrow\downarrow}(\bar{\mathbf{k}}) - P_{\uparrow\downarrow}(0)]\Lambda_{\uparrow\downarrow}(\bar{\mathbf{k}}) \\ &\quad + [\tilde{\Lambda}_{\uparrow\downarrow}(0)P_{\uparrow\downarrow}(0)\delta\gamma_{\uparrow\downarrow}(\bar{\mathbf{k}}) + \tilde{\Lambda}_{\uparrow\downarrow}(0)P_{\uparrow\downarrow}(0)\delta\gamma_{\uparrow\downarrow}(\bar{\mathbf{k}})]P_{\uparrow\downarrow}(\bar{\mathbf{k}})\Lambda_{\uparrow\downarrow}(\bar{\mathbf{k}}) \\ &\quad + [\tilde{\Lambda}_{\uparrow\downarrow}(0)P_{\uparrow\downarrow}(0)\delta\gamma_{\uparrow\downarrow}(\bar{\mathbf{k}}) + \tilde{\Lambda}_{\uparrow\downarrow}(0)P_{\uparrow\downarrow}(0)\delta\gamma_{\uparrow\downarrow}(\bar{\mathbf{k}})]P_{\uparrow\downarrow}(\bar{\mathbf{k}})\Lambda_{\uparrow\downarrow}(\bar{\mathbf{k}}) , \end{aligned} \quad (40)$$

and

$$\begin{aligned} \pi_{\downarrow\downarrow}(\bar{\mathbf{k}}) - \pi_{\downarrow\downarrow}(0) &= \tilde{\Lambda}_{\downarrow\downarrow}(0)[P_{\downarrow\downarrow}(\bar{\mathbf{k}}) - P_{\downarrow\downarrow}(0)]\Lambda_{\downarrow\downarrow}(\bar{\mathbf{k}}) + \tilde{\Lambda}_{\downarrow\downarrow}(0)[P_{\downarrow\downarrow}(\bar{\mathbf{k}}) - P_{\downarrow\downarrow}(0)]\Lambda_{\downarrow\downarrow}(\bar{\mathbf{k}}) \\ &\quad + [\tilde{\Lambda}_{\downarrow\downarrow}(0)P_{\downarrow\downarrow}(0)\delta\gamma_{\downarrow\downarrow}(\bar{\mathbf{k}}) + \tilde{\Lambda}_{\downarrow\downarrow}(0)P_{\downarrow\downarrow}(0)\delta\gamma_{\downarrow\downarrow}(\bar{\mathbf{k}})]P_{\downarrow\downarrow}(\bar{\mathbf{k}})\Lambda_{\downarrow\downarrow}(\bar{\mathbf{k}}) \\ &\quad + [\tilde{\Lambda}_{\downarrow\downarrow}(0)P_{\downarrow\downarrow}(0)\delta\gamma_{\downarrow\downarrow}(\bar{\mathbf{k}}) + \tilde{\Lambda}_{\downarrow\downarrow}(0)P_{\downarrow\downarrow}(0)\delta\gamma_{\downarrow\downarrow}(\bar{\mathbf{k}})]P_{\downarrow\downarrow}(\bar{\mathbf{k}})\Lambda_{\downarrow\downarrow}(\bar{\mathbf{k}}) . \end{aligned} \quad (41)$$

[In Eqs. (39)–(41) $\tilde{\Lambda}$ is the transpose of Λ .] The great simplification of Eqs. (39)–(41) is immediately recognized when we focus only on the b coefficients. Then

$$\begin{aligned} b_{\uparrow\uparrow} &= \text{tr}_p [\Lambda_{\uparrow\uparrow}^p(0)R_{\uparrow\uparrow}^2(p)\Lambda_{\uparrow\uparrow}^p(0) + \Lambda_{\uparrow\uparrow}^p(0)R_{\uparrow\uparrow}^2(p)\Lambda_{\uparrow\uparrow}^p(0)] \\ &\quad + \text{tr}_p \text{tr}_{p'} \left[\frac{dS_{\uparrow}}{d\mu_{\uparrow}}(p) \left(\gamma_{\uparrow\uparrow}^2(p, p') \frac{dS_{\uparrow}(p')}{d\mu_{\uparrow}} + \gamma_{\uparrow\uparrow}^2(p, p') \frac{dS_{\uparrow}}{d\mu_{\uparrow}}(p') \right) \right. \\ &\quad \left. + \frac{dS_{\uparrow}}{d\mu_{\uparrow}}(p) \left(\gamma_{\uparrow\uparrow}^2(p, p') \frac{dS_{\uparrow}}{d\mu_{\uparrow}}(p') + \gamma_{\uparrow\uparrow}^2(p, p') \frac{dS_{\uparrow}}{d\mu_{\uparrow}}(p') \right) \right] , \end{aligned} \quad (42)$$

$$\begin{aligned} b_{\uparrow\downarrow} &= \text{tr}_p [\Lambda_{\uparrow\downarrow}^p(0)R_{\uparrow\downarrow}^2(p)\Lambda_{\uparrow\downarrow}^p(0) + \Lambda_{\uparrow\downarrow}^p(0)R_{\uparrow\downarrow}^2(p)\Lambda_{\uparrow\downarrow}^p(0)] \\ &\quad + \text{tr}_p \text{tr}_{p'} \left[\frac{dS_{\uparrow}}{d\mu_{\uparrow}}(p) \left(\gamma_{\uparrow\downarrow}^2(p, p') \frac{dS_{\uparrow}(p')}{d\mu_{\uparrow}} + \gamma_{\uparrow\downarrow}^2(p, p') \frac{dS_{\uparrow}(p')}{d\mu_{\uparrow}} \right) \right. \\ &\quad \left. + \frac{dS_{\uparrow}}{d\mu_{\uparrow}}(p) \left(\gamma_{\uparrow\downarrow}^2(p, p') \frac{dS_{\uparrow}(p')}{d\mu_{\uparrow}} + \gamma_{\uparrow\downarrow}^2(p, p') \frac{dS_{\uparrow}}{d\mu_{\uparrow}}(p') \right) \right] , \end{aligned} \quad (43)$$

$$\begin{aligned} b_{\downarrow\downarrow} &= \text{tr}_p [\Lambda_{\downarrow\downarrow}^p(0)R_{\downarrow\downarrow}^2(p)\Lambda_{\downarrow\downarrow}^p(0) + \Lambda_{\downarrow\downarrow}^p(0)R_{\downarrow\downarrow}^2(p)\Lambda_{\downarrow\downarrow}^p(0)] \\ &\quad + \text{tr}_p \text{tr}_{p'} \left[\frac{dS_{\downarrow}}{d\mu_{\downarrow}}(p) \left(\gamma_{\downarrow\downarrow}^2(p, p') \frac{dS_{\downarrow}(p')}{d\mu_{\downarrow}} + \gamma_{\downarrow\downarrow}^2(p, p') \frac{dS_{\downarrow}}{d\mu_{\downarrow}}(p') \right) \right. \\ &\quad \left. + \frac{dS_{\downarrow}}{d\mu_{\downarrow}}(p) \left(\gamma_{\downarrow\downarrow}^2(p, p') \frac{dS_{\downarrow}}{d\mu_{\downarrow}}(p') + \gamma_{\downarrow\downarrow}^2(p, p') \frac{dS_{\downarrow}}{d\mu_{\downarrow}}(p') \right) \right] . \end{aligned} \quad (44)$$

In Eqs. (42)–(44),

$$\text{tr}_p(\dots) \equiv \int \frac{d^4p}{(2\pi)^4} (\dots) , \quad (45)$$

and, e.g.,

$$R_{\uparrow\uparrow}(\bar{\mathbf{k}}) = R_{\uparrow\uparrow}^0(p) + R_{\uparrow\uparrow}^2(p)\bar{\mathbf{k}}^2 + \dots , \quad (46)$$

$$\gamma_{\uparrow\uparrow}(\bar{\mathbf{k}}) = \gamma_{\uparrow\uparrow}^0(p, p') + \gamma_{\uparrow\uparrow}^2(p, p')\bar{\mathbf{k}}^2 + \dots , \quad (47)$$

$$\Lambda_{\uparrow\uparrow}^p(0) = \frac{dS_{\uparrow}^{-1}}{d\mu_{\uparrow}}(p) \equiv \frac{\partial S_{\uparrow}^{-1}}{\partial p_0}(p) + \frac{\partial S_{\uparrow}^{-1}}{\partial \mu_{\uparrow}}(p) . \quad (48)$$

μ_{\uparrow} and μ_{\downarrow} are the chemical potential of spin up and down, respectively.

These *exact* relations for b (and hence for B^{xc}) are obviously very convenient as the complicated equations describing the (two-body) electron-hole correlation has been reduced, as far as possible, in terms of the one-electron propagators and their derivatives.

Finally, we note that even with the above relations, an extension of b to metallic densities is a formidable task. However, previous analysis applied to a single component⁶ clearly demonstrates that the above relations will allow a *first-fundamental* study of B^{xc} for a spin-polarized system at metallic densities.

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