Superconductivity from long-range interaction: A crossover between the electron gas and the lattice model

Seiichiro Onari,* Ryotaro Arita,[1,†] Kazuhiko Kuroki,[2] and Hideo Aoki
Department of Physics, University of Tokyo, Hongo, Tokyo 113-0033, Japan
[1]*Max Planck Institute for Solid State Research, Heisenbergstr. 1, Stuttgart 70569, Germany*
[2]*Department of Applied Physics and Chemistry, University of Electro-Communications, Chofu, Tokyo 182-8585, Japan*
(Received 25 August 2005; revised manuscript received 13 October 2005; published 27 January 2006)

We explore how the superconductivity arising from the on-site electron-electron repulsion changes when the repulsion is made long-ranged, $1/r$-like interaction by introducing an extended Hubbard model with the repulsion extended to distant (12th) neighbors. With a simplified fluctuation-exchange approximation, we have found for the square lattice that: (i) As the band filling becomes dilute enough, the charge susceptibility becomes comparable with the spin susceptibility, where p- and then s-wave pairings become relatively dominant, in agreement with the result for the electron gas by Takada, while (ii) the d wave, which reflects the lattice structure, dominates well away from the half-filling. All of these can be understood in terms of the spin and charge structures along with the shape and size of the Fermi surface.

DOI: 10.1103/PhysRevB.73.014526 PACS number(s): 74.20.Mn

I. INTRODUCTION

While the discovery of high-T_c cuprates has kicked off intensive studies of electron mechanisms of superconductivity, these have been primarily focused on the pairing from *short-ranged* electron-electron repulsion. This is a reasonable assumption for transition metal compounds, since the main interaction between the d electrons should be short-ranged, as captured in the Hubbard model with an on-site repulsion. However, if we go back to the history of electron mechanisms of superconductivity, there is an important predecessor—the electron gas with the long-range Coulomb interaction, one of the most fundamental problems in the condensed-matter physics. The problem has a long history, where Kohn and Luttinger,[1] as early as in the 1960's, suggested that normal states in the electron gas should become unstable in favor of a superconducting state, which was later proved when the gas was dilute enough.[2] There are two important factors that discriminate the electron gas from electron systems with short-range interactions. One is that the gas becomes more strongly interacting (i.e., larger ratio of the interaction to the kinetic energy) for the more dilute concentrations. More importantly, the long-range interaction can make the *charge fluctuations* as large as the spin fluctuations as contrasted with systems with short-range interactions where the spin fluctuations dominate, so that the fluctuation-mediated interaction should change with the range of the interaction. Long-range Coulomb interaction has been recognized to be important in some classes of materials, e.g., π electron systems in organic materials, where long-range interactions, such as the Ohno potential, are often employed.

A fascinating question then is: What will become of the superconductivity in the electron system with short-range repulsions when the interaction range is increased to approach $1/r$? Besides the interaction range, there is another essential question: In lattice systems, the band filling n is a crucial parameter with the half-filling being a special point, which controls Mott's metal-insulator transition as well as the Fermi surface nesting, which in turn dominates the spin fluctuation. Indeed, we have a d-wave pairing mediated by spin fluctuations in the on-site Hubbard model around the half-filling, as theoretically suggested with, among other methods, the quantum Monte Carlo method,[3] the fluctuation exchange FLEX and dynamical cluster approximation (DCA) approximation,[4–7] and the dynamical cluster approximation.[8] By contrast, the electron gas in a continuous space, only characterized by the electron concentration (or, more precisely, r_s, the mean electron separation measured by the Bohr radius) with a circular Fermi surface, has no such special fillings. Takada[9] intensively studied superconductivity in the three-dimensional electron gas, and concluded that a p-wave pairing should occur for $r_s > 3.3$, which gives way to an s-wave pairing when the gas becomes more dilute ($r_s > 8.6$), where the pairing is interpreted to arise from charge fluctuations including plasmons.[10]

One step toward the increased range of interaction is to consider the extended Hubbard model which takes into account the nearest-neighbor repulsion V. The extended Hubbard model has been studied with various theoretical methods.[11–24] For instance, Refs. 20 and 21 address, with FLEX, the question of how the enhanced charge fluctuations in the presence of V should affect the dominant pairing symmetry, where the result indicates that a triplet pairing—as well as singlet ones—appears in the phase diagram, whose mechanism can be traced back to the structure in the charge and spin susceptibilities.

Given this background, the purpose of the present work is to explore what happens to the pairing symmetry as we make the interaction more long ranged and closer to the Coulombic interaction. For this purpose, we take a model where the interaction is extended to distant (up to the 12th here) neighbors for the square lattice, which is studied with a simplified FLEX. We then question: (i) To what extent do the effects of the lattice persist as we go away from the half-filling, and (ii) how does the pairing cross over to the pairing in the electron gas in the dilute regime? We shall show that: (i) The pairing

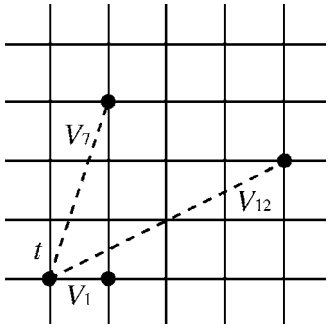

FIG. 1. A square lattice with the long-range repulsion V_n.

symmetries ($d_{x^2-y^2}$, d_{xy}) reflecting lattice structure persist well away ($n \gtrsim 0.2$) from the half-filled band, and (ii) in the dilute ($n \lesssim 0.2$) regime, the pairing symmetries are p and s in agreement with those for the electron gas. The key factors controlling the dominant symmetries are identified to be the structure (peak positions, intensities, and widths) of the charge and spin susceptibilities (along with the size of the Fermi surface in the dilute regime).

II. FORMULATION

We first introduce an extended Hubbard model with long-range interactions (Fig. 1),

$$\mathcal{H} = -t\sum_{ij}^{\mathrm{nn}}\sum_{\sigma} c_{i\sigma}^{\dagger}c_{j\sigma} + U\sum_{i} n_{i\uparrow}n_{i\downarrow} + \frac{1}{2}\sum_{ij}\sum_{\sigma\sigma'} V_{ij}n_{i\sigma}n_{j\sigma'}, \tag{1}$$

where $t(=1)$ is the nearest-neighbor transfer, taken to be the unit of energy, and the off-site Coulomb repulsion V_{ij} extends up to the 12th neighbor for the square lattice. As depicted in Fig. 1, the magnitude of the nth-neighbor repulsion $V_n = V_{|i-j|}$ is taken to be inversely proportional to the distance (e.g., $V_{12} = V/\sqrt{20}$, with $V_1 \equiv V$).

We have previously extended[21] the FLEX formalism to the extended Hubbard model with the nearest-neighbor interaction, but it is difficult to extend this beyond the second neighbors. So, here we employ a simplified FLEX, where full bubble diagrams and restricted ladder diagrams (that include only the U term) are considered for the effective interaction in a self-consistent manner. So this is a kind of random phase approximation (RPA) with all the Green's functions dressed, which was adopted in Refs. 17 and 18 for the extended Hubbard model with the nearest-neighbor interaction. We have only taken the particle-hole ladder diagrams, because we have checked that the particle-particle diagrams have a negligible influence on the self-energy, and hence on the pairing symmetry. The simplified FLEX still belongs to "conserving approximations" formulated by Baym and Kadanoff.[25,26] The FLEX neglects vertex corrections, but it has been known that the correction can lead to some problems in self-consistent calculations, especially in the dilute regime.[27] So, here we adopt the FLEX, and assume that the vertex correction would not significantly affect the competition between different pairing symmetries (although T_c, not discussed here, may be affected).

The spin (χ_{sp}) and charge (χ_{ch}) susceptibilities are then $\chi_{\mathrm{sp}}(q) = \bar{\chi}(q)/[1 - U\bar{\chi}(q)]$, $\chi_{\mathrm{ch}}(q) = \bar{\chi}(q)/\{1 + [U + 2V(q)]\bar{\chi}(q)\}$, where the irreducible susceptibility is given by $\bar{\chi}(q) = -(T/N)\Sigma_k G(k+q)G(k)$. Here $q \equiv (\mathbf{q}, \epsilon_n)$ with $\epsilon_n \equiv 2n\pi T$ being the Matsubara frequencies for bosons and $k \equiv (\mathbf{k}, \omega_n)$ with $\omega_n = (2n-1)\pi T$ for fermions, and $V(q) = 2V_1(\cos q_x + \cos q_y) + 4V_2(\cos q_x \cos q_y) + 2V_3(\cos 2q_x + \cos 2q_y) + \cdots$. The self-energy is given as

$$\Sigma(k) = \frac{T}{N}\sum_{k'}\left\{ -V(k-k') + \frac{3}{2}U^2\chi_{\mathrm{sp}}(k-k') + \left[\frac{1}{2}U^2 + 2UV(k-k') + 2V^2(k-k')\right]\chi_{\mathrm{ch}}(k-k')\right\} \times G(k'). \tag{2}$$

The gap function ϕ and T_c are obtained with Éliashberg's equation:

$$\lambda\phi(k) = -\frac{T}{N}\sum_{k'}\Gamma(k-k')G(k')G(-k')\phi(k'), \tag{3}$$

where $\lambda = 1$ corresponds to $T = T_c$, and the pairing interactions Γ_s (Γ_t) for the singlet (triplet) channels are

$$\Gamma_s(q) = U + V(q) + \frac{3}{2}U^2\chi_{\mathrm{sp}} - \left[\frac{1}{2}U^2 + 2UV(q) + 2V^2(q)\right]\chi_{\mathrm{ch}}(q), \tag{4}$$

$$\Gamma_t(q) = V(q) - \frac{1}{2}U^2\chi_{\mathrm{sp}} - \left[\frac{1}{2}U^2 + 2UV(q) + 2V^2(q)\right]\chi_{\mathrm{ch}}(q). \tag{5}$$

Here, we take $N = 32 \times 32$ **k**-point meshes and the Matsubara frequencies ω_n from $-(2N_c - 1)\pi T$ to $(2N_c - 1)\pi T$ with $N_c = 16\,384$, $T = 0.01$, and $U = 4.0$.

III. RESULT

We first show the eigenvalue, λ, of Éliashberg's equation, along with the charge (χ_{ch}) and spin (χ_{sp}) susceptibilities against the band filling n for $V = 1.0$ in Fig. 2. While λ for $T = 0.01$ is still much smaller than unity, it is difficult to go down to lower temperatures, given a huge computational demand for the long-range model. So, we assume that the dominant pairing symmetry is the one that has the largest λ at $T = 0.01$. This amounts to assuming that, while the position of boundary may shift as $T \to 0$, the order in which pairing symmetries dominate does not change. The result shows that the dominant pairing becomes $d_{x^2-y^2} \to d_{xy} \to p \to s$ as the band filling is decreased from the half-filling. Figure 3 depicts these gap functions in **k** space for typical values of n.

To explore why the dominant gap symmetry changes in such a way, we have plotted the charge and spin susceptibilities in **k** space in Fig. 4. Let us start with the region $0.8 \gtrsim n \gtrsim 0.3$, where the symmetry changes from $d_{x^2-y^2}$ to d_{xy} as n is decreased. For $n = 0.8$, the peak positions in the spin

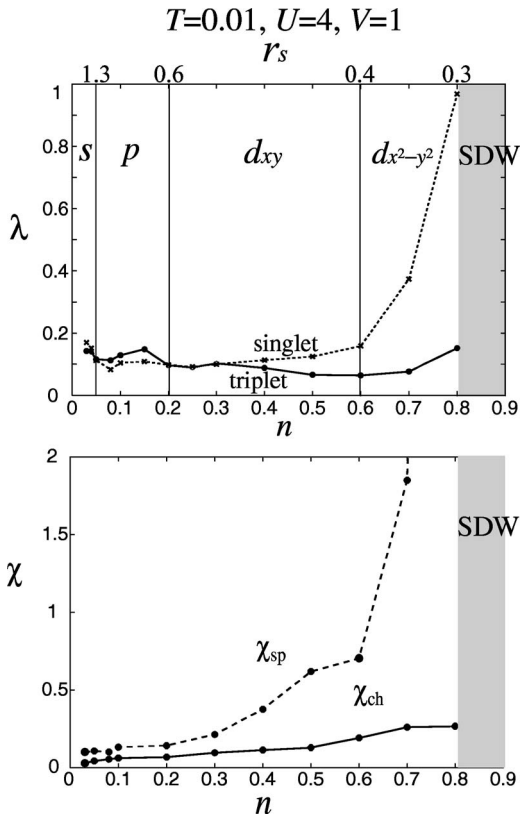

FIG. 2. (Top) Maximum eigenvalue, λ, of Éliashberg's equation in the triplet (solid line) and singlet (dotted) channels against the band filling n with the dominant symmetry indicated along with the corresponding values of r_s on the top axis. The spin density wave (SDW) phase is identified from the divergence of the spin susceptibility. (Bottom) Charge (solid line) and spin (dashed) susceptibilities against n.

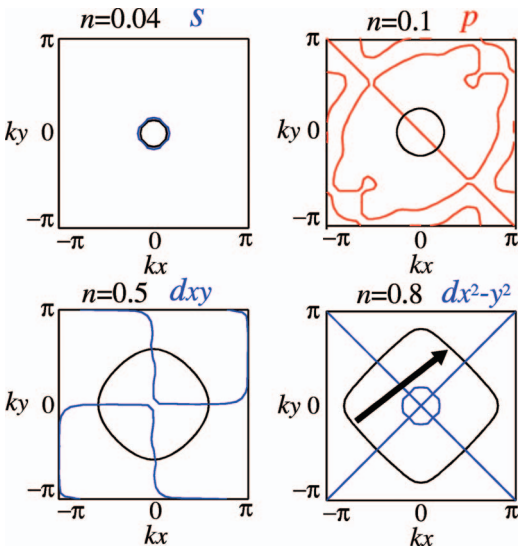

FIG. 3. (Color) Fermi surface (obtained as $\epsilon^0_{\mathbf{k}}+\mathrm{Re}\Sigma(\mathbf{k})=\mu$; black line) and nodes in the dominant gap function (blue lines for singlet pairs and red for triplet) for $0.04\leqslant n\leqslant 0.8$ with $U=4.0$ and $V=1.0$. The arrow indicates the main scattering process mediated by spin fluctuations.

susceptibility are situated around $\mathbf{k}=(\pi,\pi)$ as marked with an arrow in Fig. 4, which accounts for the $d_{x^2-y^2}$ pairing. For $n=0.5$, the peaks shift to $(0,\pm\pi)$, $(\pm\pi,0)$, which should be why the d_{xy} gap function, which changes sign across the pair hopping $(0,\pm\pi)$, $(\pm\pi,0)$, takes over.

If we further decrease the band filling, we see from Fig. 2 that χ_{ch}, which is originally much smaller than χ_{sp} for $n>0.3$, becomes comparable with χ_{sp}. When the spin-fluctuation-mediated interaction is dominant (as is the case with short-range repulsions), the singlet pairing interaction Γ_s [Eq. (4)] has the χ_{sp}-term whose coefficient is three times larger in magnitude than that for the triplet, Γ_t [Eq. (5)]. So the singlet superconductivity is generally favored when the interaction is short ranged (i.e., the spin fluctuation is dominant). Conversely, if spin and charge susceptibilities are comparable, the situation may be reversed, which indeed occurs for the triplet p-wave around $0.2\gtrsim n\gtrsim 0.05$.

In the most dilute regime ($n\lesssim 0.05$), an s-wave has the largest λ. Since the ratio of $\chi_{\mathrm{ch}}/\chi_{\mathrm{sp}}$ does not drastically change in this region, the enhancement of s requires an explanation. Here, we can note another factor that affects the pairing. This is a very general observation that nodes in the gap function, even when they are necessary to realize anisotropic pairs, act to lower T_c, since some of the pair scatterings around each node work against the paired state. In the present context, this occurs for the p wave for which the Fermi surface shrinks with decreasing n, so that the fraction of the phase space volume for the unfavorable region around the nodes increases. We identify this to be the reason why p gives way to s in the most dilute region. The competition between s and p when the range of interaction is varied is displayed in Fig. 5, where we see that correlation for s-wave is enhanced as the interaction becomes longer-ranged. We can understand this in terms of the pairing interaction: the spin structure in this regime is peaked at $\mathbf{k}=0$, which inhibits the singlet s and assists the triplet p, and the peak rapidly decreases as the range is increased. We can note in passing that, while the range of the interaction has a profound effect in the dilute regime, where the correlation for s wave is enhanced only for the long-range Coulomb interaction, a change in the interaction range in other regions only slightly shifts the boundary between different pairing symmetries.

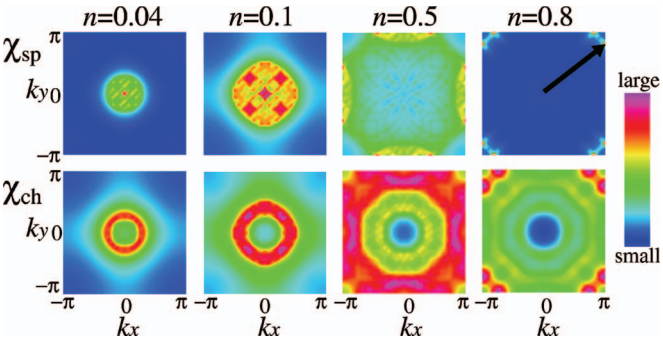

FIG. 4. (Color) Spin susceptibility χ_{sp} (top panels) and charge susceptibility χ_{ch} (bottom) in $\mathbf{k}$ space for typical values of the band filling n. To make the peaks clearer, the color coding differs from frame to frame.

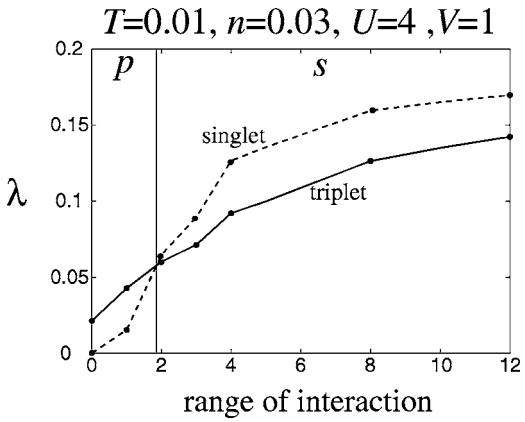

FIG. 5. The maximum eigenvalue of Éliashberg's equation for triplet (solid line) and for singlet (dotted) against the range of the interaction (in units of the lattice constant) for $n=0.03$ and $V=1.0$.

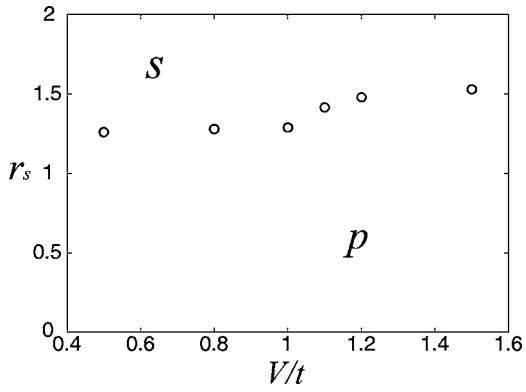

FIG. 6. The critical value of r_s between s and p waves plotted against V/t for $U=4.0$ at $T=0.01$.

IV. DISCUSSION AND SUMMARY

Let us finally compare the present result with the situation in the electron gas. Takada[9] has obtained, with the Kukkonen-Overhauser method,[28] a phase diagram as a function of the electronic-density parameter r_s for the electron gas, where the p wave (at $r_s=3.3$) and then s wave (at $r_s=8.6$) are dominant as r_s is increased (i.e., as the gas becomes more dilute). To quantify the connection between the electron gas and the present lattice model, we have to define r_s for the latter. In the effective-mass sense, we have $r_s=\sqrt{2}/(a_B^* k_F)$, where $a_B^*=(4\pi\epsilon_0\hbar^2)/(m^* e^2)$ is the effective Bohr radius, and $m^* \sim \hbar^2/(2a^2 t)$ is the effective mass with a being the lattice constant. Still, the definition can be a bit tricky, since the interaction is not truly $1/r$. Here, we eliminate e from the above equation and $V=e^2/(4\pi\epsilon_0 a)$ to define $r_s \equiv V/(\sqrt{2}ak_F t)$, where k_F is the radius of the Fermi circle when the band is dilute, while for n close to half-filling we define k_F as the largest radial distance from Γ as a measure of the Fermi surface. The values of r_s thus defined are indicated on the top axis in Fig. 2.

We first examine how the boundary value of r_s between s and p waves changes with V in Fig. 6. We can see that the boundary is almost flat, especially for $V/t \leqslant 1$, where the dispersion around small k_F is close to those of the electron gas. So the result is consistent in that the phase is basically determined by r_s alone as in the electron gas.

While p and s waves are dominant in the dilute concentration regime in both of the present and electron-gas[9] models, the boundary values of r_s exhibit significant differences between the two. One factor for the discrepancy should be that the present model is a two-dimensional system, while Ref. 9 considers three-dimensional systems. In the plasmon-mechanism analysis of superconductivity[10] the critical r_s in two dimensions is seen to be much reduced (by about one-third) from that for three dimensions. Moreover, the present model differs from the Coulomb gas even though the 12th neighbor interaction is included, since a cutoff in the interaction should degrade Gauss's law (hence degrade the plasmon modes). Extending our model to three dimensions may cast a light on this.

ACKNOWLEDGMENTS

We thank Yasutami Takada for illuminating comments. This work is in part supported by a Grant-in-Aid for Science Research on Priority Area from the Japanese Ministry of Education. Numerical calculations were performed at the supercomputer center, ISSP.

*Present address: Department of Applied Physics, Nagoya University, Chikusa, Nagoya 464-8603, Japan.

†On leave of absence from Department of Physics, University of Tokyo, Hongo, Tokyo 113-0033, Japan.

[1] W. Kohn and J. Luttinger, Phys. Rev. Lett. **15**, 524 (1965).
[2] A. V. Chubukov, Phys. Rev. B **48**, 1097 (1993).
[3] K. Kuroki and H. Aoki, Phys. Rev. B **56**, R14287 (1997).
[4] N. E. Bickers, D. J. Scalapino, and S. R. White, Phys. Rev. Lett. **62**, 961 (1989).
[5] N. E. Bickers and D. J. Scalapino, Ann. Phys. **193**, 206 (1989).
[6] T. Dahm and L. Tewordt, Phys. Rev. B **52**, 1297 (1995).
[7] M. Langer, J. Schmalian, S. Grabowski, and K. H. Bennemann, Phys. Rev. Lett. **75**, 4508 (1995).
[8] T. A. Maier, M. Jarrell, T. C. Schulthess, P. R. C. Kent, and J. B. White, Phys. Rev. Lett. **95**, 237001 (2005).
[9] Y. Takada, Phys. Rev. B **47**, 5202 (1993).
[10] Y. Takada, J. Phys. Soc. Jpn. **45**, 786 (1978).
[11] Y. Zhang and J. Callaway, Phys. Rev. B **39**, 9397 (1989).
[12] Z. Tešanović, A. R. Bishop, and R. L. Martin, Solid State Commun. **68**, 337 (1988).
[13] M. Murakami, J. Phys. Soc. Jpn. **69**, 1113 (2000).
[14] H. Seo and H. Fukuyama, J. Phys. Soc. Jpn. **66**, 1249 (1997).
[15] M. Onozawa, Y. Fukumoto, A. Oguchi, and Y. Mizuno, Phys. Rev. B **62**, 9648 (2000).
[16] D. J. Scalapino, E. Loh, Jr., and J. E. Hirsch, Phys. Rev. B **35**, 6694 (1987).

[17] A. Kobayashi, Y. Tanaka, M. Ogata, and Y. Suzumura, J. Phys. Soc. Jpn. **73**, 1115 (2004).
[18] Y. Tanaka, Y. Yanase, and M. Ogata, J. Phys. Soc. Jpn. **73**, 319 (2004).
[19] G. Esirgen, H. B. Schuttler, and N. E. Bickers, Phys. Rev. Lett. **82**, 1217 (1999).
[20] R. Arita, S. Onari, K. Kuroki, and H. Aoki, Phys. Rev. Lett. **92**, 247006 (2004).
[21] S. Onari, R. Arita, K. Kuroki, and H. Aoki, Phys. Rev. B **70**, 094523 (2004).
[22] J. Merino and R. H. McKenzie, Phys. Rev. Lett. **87**, 237002 (2001).
[23] K. Sano and Y. Ono, J. Phys. Chem. Solids **63**, 1567 (2002).
[24] K. Kuroki, K. Kusakabe, and H. Aoki, Phys. Rev. B **50**, 575 (1994).
[25] G. Baym and L. P. Kadanoff, Phys. Rev. **124**, 287 (1961).
[26] G. Baym, Phys. Rev. **127**, 1391 (1962).
[27] B. Holm and U. von Barth, Phys. Rev. B **57**, 2108 (1998).
[28] C. A. Kukkonen and A. W. Overhauser, Phys. Rev. B **20**, 550 (1979).