Spin-fluctuation exchange study of superconductivity in two- and three-dimensional single-band Hubbard models

Ryotaro Arita, Kazuhiko Kuroki, and Hideo Aoki
Department of Physics, University of Tokyo, Hongo, Tokyo 113-0033, Japan
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In order to identify the most favorable situation for superconductivity in the repulsive single-band Hubbard model, we have studied instabilities for *d*-wave pairing mediated by antiferromagnetic spin fluctuations and *p*-wave pairing mediated by ferromagnetic fluctuations with the fluctuation exchange approximation in both two dimensions and three dimensions. By systematically varying the band filling and band structure we have shown that (i) *d* pairing is stronger in two dimensions than in three dimensions and (ii) *p* pairing is much weaker than *d* pairing. [S0163-1829(99)04446-X]

The discovery of high-temperature superconductivity in copper oxides by Bednorz and Müller[1] has kicked off intensive studies for electron mechanisms of superconductivity. Specifically, it is becoming increasingly clear that superconductivity can arise from repulsive electron-electron interactions. A persuasive scenario is that the superconductivity comes from a pairing interaction mediated by antiferromagnetic (AF) spin fluctuations. A phenomenological calculation[2–5] along this line has succeeded in reproducing anisotropic *d*-wave superconductivity as well as anomalous normal-state properties. Analytic calculations on a microscopic level with the fluctuation exchange (FLEX) approximation, developed by Bickers *et al.*,[6] has also been applied to the Hubbard model on the two-dimensional (2D) square lattice[7,8] to show the occurrence of superconductivity. Numerically, a quantum Monte Carlo study has indicated pairing instability.[9]

These results indicate that the superconductivity near the AF instability in 2D has a ''low T_C'' $\sim O(0.01t)$ (t is the transfer integral), i.e., two orders of magnitude smaller than the original electronic energy, but still ''high T_C'' $\sim O(100\ \mathrm{K})$ for $t \sim O(1\ \mathrm{eV})$. Then the next fundamental questions, which we address in this paper, are the following: (i) Is the 2D system more favorable for spin-fluctuation-mediated superconductivity than in three dimensions (3D)? (ii) Can other pairing, such as a triplet *p* pairing in the presence of *ferromagnetic* spin fluctuations, become competitive? We take the single-band, repulsive Hubbard model as the simplest possible model, and look into the pairing with the FLEX method both in 2D and 3D. The FLEX method has the advantage that systems having large spin fluctuations can be handled.

Let us touch a little more upon the background to the above two questions. The possibility of triplet pairing mediated by ferromagnetic fluctuations has been investigated for superfluid ^{3}He,[10] the heavy fermion system UPt_3,[11] and most recently, the oxide Sr_2RuO_4.[12] It was shown that ferromagnetic fluctuations favor triplet pairing by Layzer and Fay[14] before the experimental observation of *p*-wave pairing in ^{3}He. For the electron gas model, Fay and Layzer[15] or later Chubukov[13] has extended the Kohn-Luttinger theorem[16] to *p* pairing for 2D and 3D electron gas in the dilute limit. Takada[17] discussed the possibility of *p*-wave superconductivity in the dilute electron gas with the Kukkonen-Overhauser model.[18] As for lattice systems, the 2D Hubbard model with large enough next-nearest-neighbor hopping (t') has been shown to exhibit *p* pairing for small band fillings.[19] Hlubina[20] reached a similar conclusion by evaluating the superconducting vertex in a perturbative way.[21] However, the energy scale of the *p* pairing in the Hubbard model, i.e., T_C, has not been evaluated so far.

As for 3D systems, Scalapino *et al.*[22] showed for the Hubbard model that paramagnon exchange near a spin-density-wave instability gives rise to a strong singlet *d*-wave pairing interaction, but T_C was not discussed there. Nakamura *et al.*[23] extended Moriya's spin fluctuation theory of superconductivity[3] to 3D systems, and concluded that T_C is similar between the 2D and 3D cases provided that common parameter values (scaled by the bandwidth) are taken. However, the parameters there are phenomenological ones, so we wish to see whether the result remains valid for microscopic models.

Here we shall show that (i) *d*-wave instability mediated by AF spin fluctuations in a 2D square lattice is much stronger than those in 3D, while (ii) *p*-wave instability mediated by ferromagnetic spin fluctuations in 2D are much weaker than the *d* instability. These results, which cannot be predicted *a priori*, suggest that for the Hubbard model the ''best'' situation for the pairing instability is the 2D case with dominant AF fluctuations.

We consider the single-band Hubbard model with transfer energy $t_{ij}=t$ $(=1$ hereafter) for nearest neighbors along with $t_{ij}=t'$ for second-nearest neighbors, which is included to incorporate the band structure dependence. The FLEX approximation starts from a set of skeleton diagrams for the Luttinger-Ward functional to generate a (k-dependent) self-energy based on the idea of Baym and Kadanoff.[24] Hence the FLEX approximation is a self-consistent perturbation approximation with respect to on-site interaction U.

To obtain T_C, we solve, with the power method,[6] the eigenvalue (Éliashberg) equation

$$\lambda \Sigma^{(2)}(k) = \frac{T}{N} \sum_{k'} \Sigma^{(2)}(k') |G(k')|^2 V^{(2)}(k-k'), \quad (1)$$

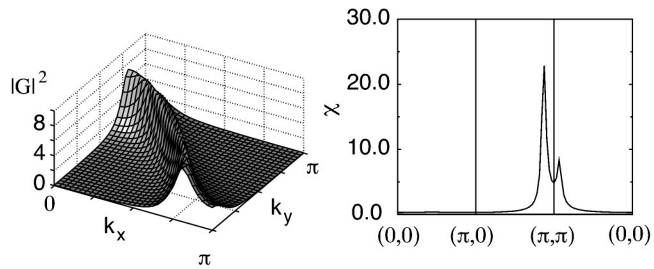

FIG. 1. The squared absolute value of the Green's function for the smallest Matsubara frequency, $i\omega_n = i\pi k_B T$ (left), and the random phase approximation (RPA) spin susceptibility (right) against the wave number for the 2D Hubbard model with $t'=0$, $n=0.85$, and $U=4$.

where

$$V^{(2)}(q) = \frac{1}{2}\left[\frac{U^2\chi_0(q)}{1+U\chi_0(q)}\right] - \frac{3}{2}\left[\frac{U^2\chi_0(q)}{1-U\chi_0(q)}\right] \tag{2}$$

for spin singlet pairing and

$$V^{(2)}(q) = \frac{1}{2}\left[\frac{U^2\chi_0(q)}{1+U\chi_0(q)}\right] + \frac{1}{2}\left[\frac{U^2\chi_0(q)}{1-U\chi_0(q)}\right] \tag{3}$$

for spin triplet pairing, where $\chi_0(q) \equiv -T/N\Sigma_k G(k)G(k+q)$ is the irreducible susceptibility, $G(k)$ the dressed Green's function, and $\Sigma^{(2)}(k)$ the anomalous self-energy. At $T=T_C$, the maximum eigenvalue $\lambda_{\rm Max}$ reaches unity. We take $N=64^2$ sites with $n_c=2048$ Matsubara frequencies for 2D, or $N=32^3$ with $n_c=1024$ for 3D.

Let us start with the 2D case having strong AF fluctuations. In Fig. 1, we plot $\chi_{\rm RPA}(q) = \chi_0/(1-U\chi_0)$ as a function of momentum for the 2D Hubbard model with $t'=0$, $n=0.85$ (nearly half-filled) with $U=4$ and $T=0.03$. A dominant AF spin fluctuation is seen from $\chi_{\rm RPA}$ peaked near (π,π).

We can then solve the Éliashberg equation (1) to plot in Fig. 2(a) $\lambda_{\rm Max}$ as a function of temperature T (normalized by t). The behavior of $|G(k,i\pi k_B T)|^2$ that appears in the Éliashberg equation is indicated in Fig. 1. How $\lambda_{\rm Max}$ is close to unity measures the pairing, and $\lambda_{\rm Max}$ tends to unity at $T \sim 0.02$, in accordance with previous results.[7,25] We also plot the reciprocal of the peak value of $\chi_{\rm RPA}(\mathbf{k},0)$, where $1/\chi \to 0$ indicates the magnetic ordering. While we cannot compare $\lambda_{\rm Max}$ and $\chi_{\rm RPA}$ on an equal footing, since pairing fluctuations are neglected in the Éliashberg equation while the susceptibility is treated beyond the mean field, we can discuss the behavior of $\lambda_{\rm Max}$ when the situation is varied.

Keeping the above result in mind as a reference, we move on to the case with ferromagnetic spin fluctuations, where triplet pairing is expected. This situation can be realized for relatively large t' (~ 0.5) and electron density away from half-filling in the 2D Hubbard model. Physically, the van Hove singularity shifts toward the band bottom with t', and the large density of states at the Fermi level for the dilute case favors ferromagnetism. It has in fact been shown from a quantum Monte Carlo study that the ground state is fully spin polarized at $t'=0.47$, $n\sim 0.4$.[26,20]

We have calculated $\lambda_{\rm Max}$ for the density varied over $0.2 \leq n \leq 0.6$ and t' varied over $0.3 \leq t' \leq 0.6$ for $U=4,6$ with

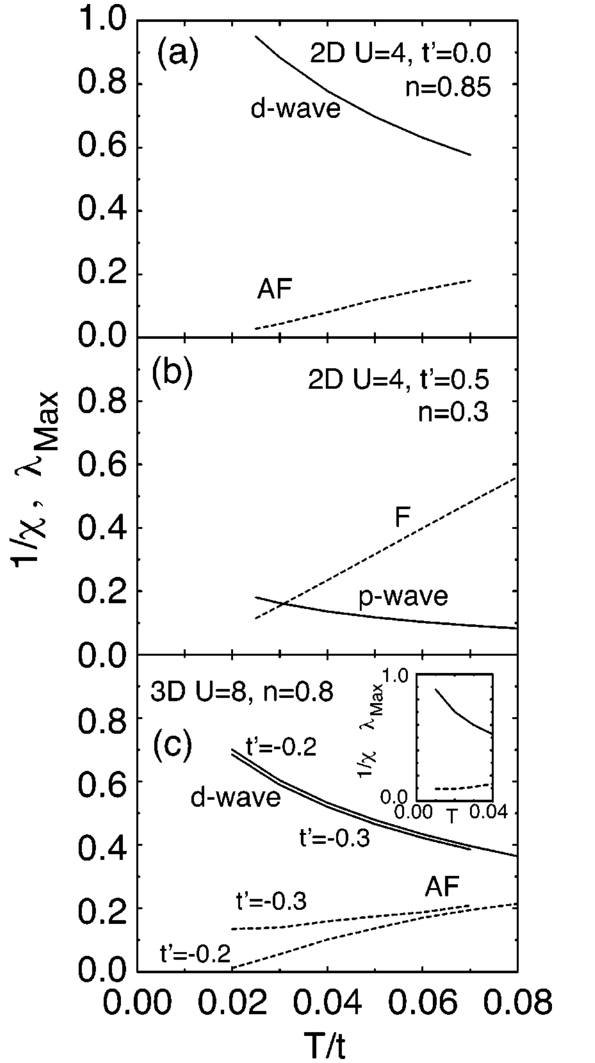

FIG. 2. The maximum eigenvalue of the Éliashberg equation (solid lines) and the reciprocal of the peak of $\chi_{\rm RPA}$ (either ferromagnetic or antiferromagnetic, dashed lines) against temperature for the Hubbard model in (a) 2D with $t'=0$, $n=0.85$, and $U=4$, (b) 2D with $t'=0.5$, $n=0.3$, and $U=4$, and (c) 3D with $t'=-0.2,-0.3$, $n=0.8$, and $U=8$. The inset in (c) is the results for a larger number of Matsubara frequencies (=2048) for $t'=-0.3$.

$T=0.03$, and have found that $\lambda_{\rm Max}$ becomes largest for $n=0.3$, $t'=0.5$, so we concentrate on this parameter set hereafter. If we look at in Fig. 3 the momentum dependence of $|G(k,i\pi k_B T)|^2$ and $\chi_{\rm RPA}$ for this case with $U=4$, $\chi_{\rm RPA}$ is indeed peaked at Γ [$\mathbf{k}=(0,0)$]. The question then is the be-

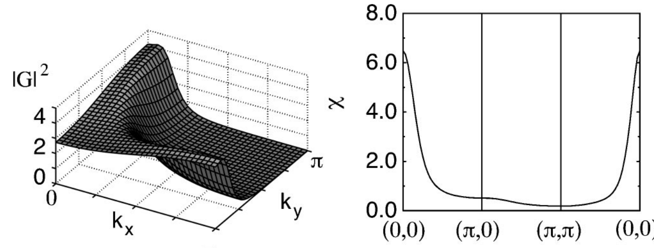

FIG. 3. A similar plot as in Fig. 1 for the 2D Hubbard model for a finite $t'=0.5$ with a smaller $n=0.3$ with $U=4$.

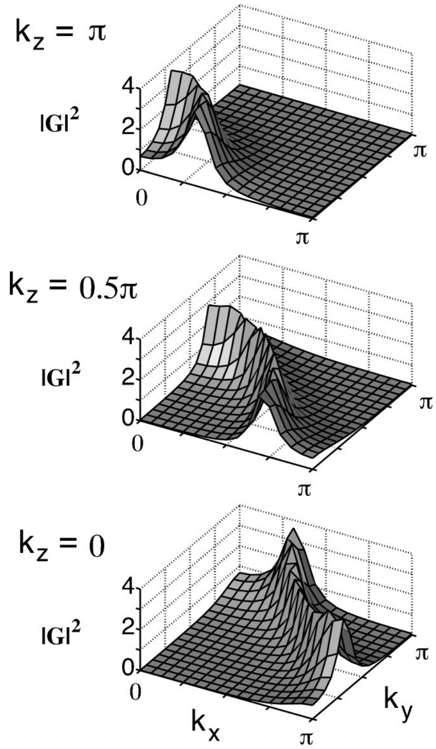

FIG. 4. A plot for the Green's function against k_x and k_y with $k_z=0,\pi/2,\pi$ for the 3D Hubbard model with $t'=-0.2$, $n=0.8$, $U=8$, and $T=0.03$.

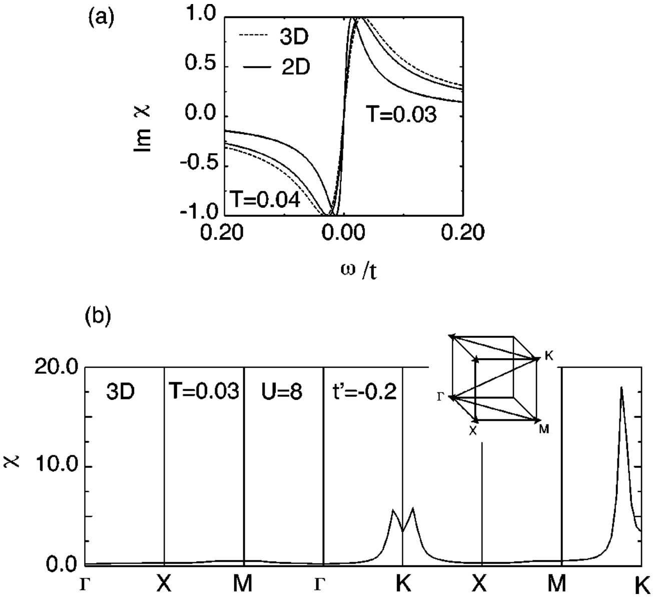

FIG. 5. (a) Im $\chi_{\mathrm{RPA}}(\mathbf{k}_{\mathrm{Max}},\omega)$ (normalized by its maximum value) as a function of ω/t for the 3D Hubbard model with $t'=-0.2$, $n=0.8$, $U=8$, and $T=0.03,0.04$ (dashed line) and for the 2D Hubbard model with $t'=0$, $n=0.85$, $U=4$, and $T=0.03,0.04$ (solid line). For $T=0.03$ 2D and 3D results almost overlap with each other. (b) RPA spin susceptibility $\chi_{\mathrm{RPA}}(\mathbf{k},0)$ as a function of the wave number for the 3D Hubbard model with $t'=-0.2$, $n=0.8$, $T=0.03$, and $U=8$.

havior of λ_{Max} as a function of T, Fig. 2(b), which shows that λ_{Max} is much smaller than that in the AF case, Fig. 2(a).

A low T_C for the ferromagnetic case contrasts with a naive expectation from the BCS picture, in which the Fermi level located around a peak in the density of states favors superconductivity. We may trace back twofold reasons why this does not apply. First, if we look at the dominant ($\propto 1/[1-U\chi_0(q)]$) term of the pairing potential $V^{(2)}$ itself in Eqs. (2) and (3), the triplet pairing interaction is only one-third of that for singlet pairing. Second, the factor $|G|^2$ for the ferromagnetic case (Fig. 3) is smaller than that in the AF case (Fig. 1), which implies that the self-energy correction is larger in the former. A larger self-energy correction (smaller $|G|^2$) leads to smaller eigenvalues of the Éliashberg equation (1). Even when we take a larger repulsion U to increase the triplet pairing attraction (susceptibility), this makes the self-energy correction even stronger, resulting in only a small change in λ.

Let us now move on to the case of d-wave pairing in the 3D Hubbard model. In this case, we find that the Γ_3^+ representation of the O_h group[27] has the largest λ_{Max}, so we look at this pairing symmetry hereafter. We have calculated λ_{Max} for the density varied over $0.75\leqslant n\leqslant 0.9$ and t' varied over $-0.5\leqslant t'\leqslant +0.4$ for $U=4,6,8,10,12$ with $T=0.03$. Among these parameter sets, we have found that λ_{Max} becomes largest for $n=0.8$, $t'=-0.2$ to -0.3, and $U=8$–10, so hereafter we concentrate on this parameter set.

In Fig. 2(c), we again plot λ_{Max} along with the reciprocal of the peak value of $\chi_{\mathrm{RPA}}(\mathbf{k},0)$ as a function of T for $t'=-0.2,-0.3$, $U=8$, and $n=0.8$. We can immediately see that the pairing tendency in 3D is much *weaker* than that in 2D. Technically, for the sample size $N=32^3$ and the number of Matsubara frequencies $n_c=1024$ there are some finite-size effects for $T<0.02$. As the inset for a larger $n_c=2048$ exemplifies, however, λ_{Max} tends to increase with N and n_c, and we believe that a finite T_C (<0.01) may be obtained at least for $t'=-0.3$, $U=8$, and $n=0.8$ in the limit of large N and n_c, but this is still significantly smaller than in 2D.

Having confirmed this, the question now is, why is the d superconductivity much stronger in 2D than in 3D? We can pinpoint the origin by looking at the various factors involved in the Éliashberg equation. Namely, we question the height of $V^{(2)}$ and $|G|^2$ along with the width of the region, both in the momentum sector and in the frequency sector, over which $V^{(2)}(k)$ contributes to the summation over $k\equiv(\mathbf{k},i\omega_n)$.

We first plot $|G|^2$ for $k_z=0,\pi/2,\pi$ as a function of k_x and k_y in the 3D Hubbard model for $t'=-0.2$, $n=0.8$ with $U=8$ in Fig. 4. We can see that the maximum of $|G|^2$ in 3D, if multiplied by U^2 arising in the Éliashberg equation, is in fact larger than in 2D. Were this factor the origin, a larger λ_{Max} would result in 3D.

We can then question how the peak in χ_{RPA} spreads in the frequency axis. Figure 5(a) displays Im $\chi_{\mathrm{RPA}}(k_{\mathrm{Max}},\omega)$ [$\mathbf{k}_{\mathrm{Max}}$ is the momentum for which $\chi(\mathbf{k},0)$ is maximum] as a function of ω (obtained by an analytic continuation with Padé approximation[28]). The figure compares the ''best 3D'' case ($t'=-0.2, n=0.8, U=8$) with a typical 2D case with $t'=0$, $n=0.85$, and $U=4$ having a similar magnitude of χ. We can see that Im $\chi(\omega)$, when this quantity is normalized by its maximum value while ω by t, exhibits surprisingly similar behaviors for 2D and 3D. So we can exclude the frequency width from the reason for the 2D-3D difference. Note that if the frequency spread of the susceptibility scaled not with t but with the *band width*, as Nakamura *et al.*[23] have assumed, λ_{Max} would have become larger. So this is one reason why we stress that the present result, that 2D is the best, is by no means readily predictable.

If we turn to the momentum sector, Fig. 5(b) for $\chi_{\mathrm{RPA}}(\mathbf{k},0)$ shows that the width a of the $\chi_{\mathrm{RPA}}(\mathbf{k},0)$ peak in each momentum direction is similar to those in 2D (Fig. 1). Since the right-hand side of the Éliashberg equation (1) is normalized by $N \propto L^D$ with L being the linear dimension of the system, $\lambda \propto (a/L)^D$ is smaller in 3D than that in 2D when the main contribution of $V^{(2)}$ to λ is confined around (π,π) or (π,π,π). So we can conclude that this is the main reason why 2D differs from 3D.

We have also obtained results (not shown here) in 3D for the body-centered-cubic lattice near half-filling (where strong AF fluctuations are expected), but the d pairing is again weak. The p pairing in the face-centered-cubic lattice with low band filling (where ferromagnetic fluctuations are expected) is found to be even weaker. These results will be published elsewhere.

To summarize, d pairing in 2D is the best situation for the repulsion-originated (i.e., spin-fluctuation-mediated) superconductivity in the Hubbard model. In this sense, the layer-type cuprates do seem to hit upon the right situation. However, our conclusion has been obtained for the simplest possible single-band Hubbard model, while the detailed behavior of T_C may depend on the model. Indeed, if we turn to other 3D superconductors, the heavy fermion system, in which the pairing is thought to be meditated by spin fluctuations, the T_C, when normalized by the bandwidth W, is known to be of the order of $0.001W$. Since the present result indicates that T_C, normalized by W, is $\sim 0.0001W$ at best in the 3D Hubbard model, we may envisage that the heavy fermion system is an instance in which larger frequency and/or momentum spreads in $\chi(\mathbf{k},\omega)$ are utilized than in the Hubbard model.

After completion of this study, we came to know the work by Monthoux and Lonzarich.[29] Using a phenomenological approach, they conclude for 2D systems that the d-wave pairing is much stronger than p-wave pairing, which is consistent with the present result.

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