

Spin susceptibility representation of the pairing interaction for the two-dimensional Hubbard model

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Using numerical dynamic cluster quantum Monte Carlo results, we study a simple approximation for the pairing interaction of a two-dimensional Hubbard model with an on-site Coulomb interaction U equal to the bandwidth. We find that with an effective temperature-dependent coupling $\bar{U}(T)$ and the numerically calculated spin susceptibility $\chi(K-K')$, the d -wave pairing interaction is well approximated by $\frac{3}{2}\bar{U}^2\chi(K-K')$.

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I. INTRODUCTION

Numerical calculations have shown that the dominant contribution to the d -wave pairing interaction in the Hubbard model comes from a spin $S=1$ channel.^{1,2} It is therefore interesting to determine how well the simple random-phase approximation (RPA) form

$$\frac{3}{2}\bar{U}^2\chi(K-K') \quad (1)$$

can describe this interaction. Here χ is the spin susceptibility, \bar{U} is an effective coupling strength, and $K=(\mathbf{K}, \omega_n)$, with $\omega_n=(2n+1)\pi T$ a fermion Matsubara frequency. Equation (1) is the form that one expects in weak coupling.³⁻⁶ However, we are interested in the case in which the Hubbard on-site Coulomb interaction U is comparable to the bandwidth, since this is the region which is believed to be appropriate for the cuprates.⁷ This is also the parameter regime in which the pairing is the strongest.² Here, for the parameters we use throughout this paper including a near-neighbor hopping $t=1$ and $U=8$, the single-particle propagator and density of states show clear evidence that one is dealing with a doped Mott system. In particular, one sees structures associated with upper and lower Hubbard bands as well as a conduction band.^{2,8} In this case, it is unclear whether the simple form given by Eq. (1) can adequately describe the pairing interaction. We believe that there are two reasons that this is possible. First, the leading contribution of U to the d -wave pairing channel vanishes due to the pairing symmetry, and secondly, the dressed spin susceptibility χ , and not the perturbative RPA form, will be used in Eq. (1).

To see how well Eq. (1) can describe the pairing interaction, we first discuss the fitting procedure which will be used to determine a temperature-dependent effective coupling $\bar{U}(T)$. Following this, we compare the d -wave eigenvalue and the \mathbf{K} and ω_n dependences of the eigenfunction of the Bethe-Salpeter equation using the interaction given by Eq. (1), with the results obtained using the “exact” interaction. Throughout this paper, “exact” will refer to numerical results obtained using a dynamic cluster approximation (DCA)

Monte Carlo technique.⁹⁻¹² We will then conclude by discussing the relationship of \bar{U} to the bare interaction.

II. FITTING THE EFFECTIVE COUPLING \bar{U}

For the traditional low T_c superconductors, the phonon-mediated s -wave pairing interaction is characterized by¹³

$$\alpha^2 F(\omega) = - \sum_{\nu} \frac{\left\langle |g_{\mathbf{p},\mathbf{p}'}^2| \frac{\Im m}{\pi} D_{\nu}(\mathbf{p}-\mathbf{p}', \omega) \delta(\varepsilon_{\mathbf{p}}) \delta(\varepsilon_{\mathbf{p}'}) \right\rangle_{\mathbf{p}\mathbf{p}'}}{\langle \delta(\varepsilon_{\mathbf{p}}) \rangle_{\mathbf{p}}}. \quad (2)$$

Here, $D_{\nu}(\mathbf{q}, \omega)$ is the phonon propagator for polarization ν and $\langle \delta(\varepsilon_{\mathbf{p}}) \rangle_{\mathbf{p}}$ represents an average over the Fermi surface weighted by a \mathbf{p} -dependent density of states which varies as $v_F^{-1}(\mathbf{p})$. The coupling strength λ is given by

$$\lambda = 2 \int_0^{\infty} d\omega \frac{\alpha^2 F(\omega)}{\omega}, \quad (3)$$

and it clearly depends on the phonon dynamics. However, by substituting Eq. (2) into Eq. (3) and making use of the usual dispersion relation, λ can be conveniently expressed in terms of the zero-frequency limit of the phonon propagator $D_{\nu}(\mathbf{q}, \omega=0)$:

$$\lambda = - \sum_{\nu} \frac{\langle |g_{\mathbf{p},\mathbf{p}'}^2| D_{\nu}(\mathbf{p}-\mathbf{p}', 0) \delta(\varepsilon_{\mathbf{p}}) \delta(\varepsilon_{\mathbf{p}'}) \rangle_{\mathbf{p}\mathbf{p}'}}{\langle \delta(\varepsilon_{\mathbf{p}}) \rangle_{\mathbf{p}}}. \quad (4)$$

At a finite temperature, $D_{\nu}(\mathbf{p}-\mathbf{p}', 0)$ is replaced by $1/2[D_{\nu}(\mathbf{p}-\mathbf{p}', 0) + D_{\nu}(\mathbf{p}-\mathbf{p}', 2\pi T)]$.

For the Hubbard model, we lack a Migdal theorem and the pairing interaction is calculated with a dynamic cluster quantum Monte Carlo algorithm.⁹⁻¹² The dynamical cluster approximation maps the original lattice model onto a periodic cluster of size N_c sites embedded in a self-consistent host. The essential assumption is that short-range quantities, such as the self-energy and its functional derivatives (the irreducible vertex functions), are well represented as diagrams constructed from the coarse-grained Green's function.

For the problem of interest, this is a reasonable assumption for systems where the correlations that mediate the pairing are short ranged. To this end, the first Brillouin zone is divided into N_c cells, with each cell represented by its center wave vector \mathbf{K} surrounded by N/N_c lattice wave vectors labeled by $\tilde{\mathbf{k}}$. The reduction of the N -site lattice problem to an effective N_c -site cluster problem is achieved by coarse-graining the single-particle Green's function; i.e., averaging $G(\mathbf{K}+\tilde{\mathbf{k}})$ over $\tilde{\mathbf{k}}$ within a cell, which converges to a cluster Green's function $G_c(\mathbf{K})$. Consequently, the compact Feynman diagrams constructed from $G_c(\mathbf{K})$ collapse onto those of an effective cluster problem embedded in a host, which accounts for the fluctuations arising from the hopping of electrons between the cluster and the rest of the system. The compact cluster quantities are then used to calculate the corresponding lattice quantities.

The pairing interaction is given by the irreducible part of the particle-particle vertex

$$\Gamma^{pp}(K;K') \equiv \Gamma^{pp}(K,-K;K',-K'), \quad (5)$$

with $K=(\mathbf{K},\omega_n)$. One can also use the DCA to calculate the spin susceptibility $\chi(\mathbf{Q},\omega_n)$.^{11,12} In an analogous manner to Eq. (4), we now introduce a d -wave coupling strength

$$-\frac{1}{2} \frac{\langle g(\mathbf{K})\Gamma_{\text{even}}^{pp}(\mathbf{K},\pi T;\mathbf{K}',\pi T)g(\mathbf{K}') \rangle_{\mathbf{K}\mathbf{K}'}}{\langle g^2(\mathbf{K}) \rangle_{\mathbf{K}}} \quad (6)$$

with the even frequency, even momentum part of the irreducible particle-particle vertex

$$\begin{aligned} \Gamma_{\text{even}}^{pp}(\mathbf{K},\pi T;\mathbf{K}',\pi T) \\ = \frac{1}{4} [\Gamma^{pp}(\mathbf{K},\pi T;\mathbf{K}',\pi T) + \Gamma^{pp}(\mathbf{K},\pi T;-\mathbf{K}',\pi T) \\ + \Gamma^{pp}(\mathbf{K},\pi T;\mathbf{K}',-\pi T) + \Gamma^{pp}(\mathbf{K},\pi T;-\mathbf{K}',-\pi T)] \end{aligned} \quad (7)$$

and $g(\mathbf{K})=(\cos K_x - \cos K_y)$. An effective coupling $\bar{U}(T)$ may then be obtained by requiring that the d -wave coupling strength in Eq. (6) is the same at a given temperature for the approximate interaction one obtains by replacing $\Gamma^{pp}(K;K')$ with the interaction in Eq. (1). In Fig. 1, we show the results for $\bar{U}(T)$ for two different DCA cluster sizes,²³ $N_c=4$ and $N_c=24$, for the case in which $U=8$ and the site filling $\langle n \rangle = 0.85$. Here, one sees that \bar{U} is smaller than U and decreases at lower temperatures. We will discuss the physics that underlies this effect after we explore how well $\frac{3}{2}\bar{U}^2\chi(K-K')$ represents $\Gamma^{pp}(K;K')$.

III. RESULTS FOR THE PARTICLE-PARTICLE BETHE-SALPETER EQUATION

The leading low-temperature eigenvalue of the particle-particle Bethe-Salpeter equation

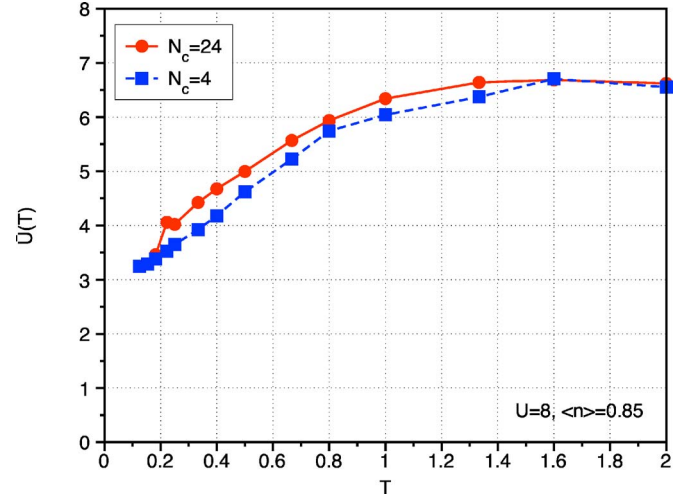


FIG. 1. (Color online) The coupling strength \bar{U} for $U=8$ in units in which $t=1$ and a site filling $\langle n \rangle = 0.85$ calculated for two cluster sizes $N_c=4$ and 24.

$$-\frac{T}{N_c} \sum_{K'} \Gamma_{\text{even}}^{pp}(K,-K;K',-K') \bar{\chi}_0^{pp}(K') \phi_\alpha(K') = \lambda_\alpha \phi_\alpha(K) \quad (8)$$

corresponds to an eigenfunction with d -wave symmetry. Here, we have coarse-grained the Green's function legs, $\bar{\chi}_0^{pp}(K') = \frac{N}{N} \sum_{\tilde{\mathbf{k}}} G_1(\mathbf{K}'+\tilde{\mathbf{k}}) G_1(-\mathbf{K}'-\tilde{\mathbf{k}})$, according to the DCA assumption. The curves with solid symbols in Fig. 2 show the d -wave eigenvalue versus T obtained from Eq. (8) with the exact DCA interaction Γ^{pp} . The curves with open symbols show the d -wave eigenvalue obtained from Eq. (8) when Γ^{pp} is replaced with $\frac{3}{2}\bar{U}^2\chi(K-K')$. Here, we are using DCA results for $\chi(K-K')$ as well as the single-particle propagator $G(\mathbf{k})$ that appears in Eq. (8). One sees that with $\bar{U}(T)$ determined as discussed in Sec. II, the temperature de-

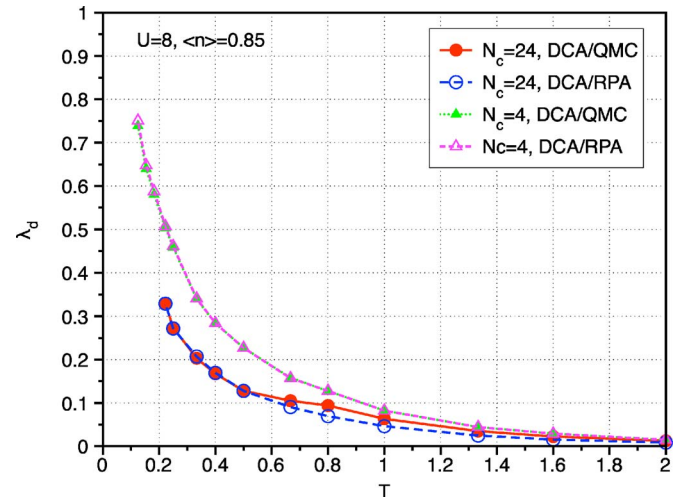


FIG. 2. (Color online) The d -wave eigenvalue versus T obtained from the RPA form [Eq. (1)] (open symbols) and from the “exact” DCA interaction (solid symbols) for $N_c=4$ and 24.

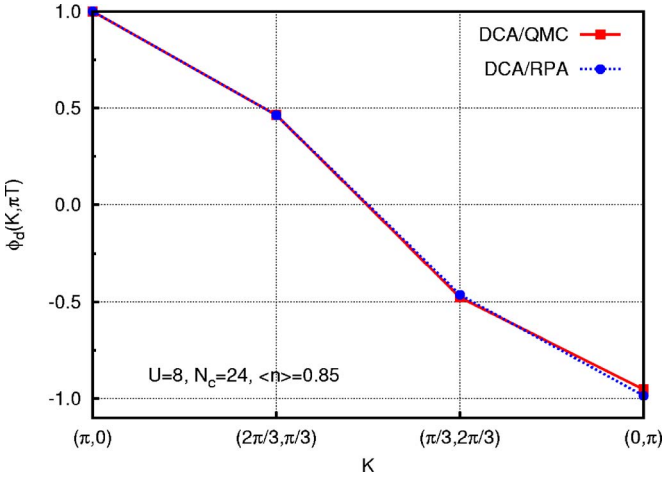


FIG. 3. (Color online) The momentum dependence of the d -wave eigenvector $\phi(\mathbf{K}, \omega_n)$ for $\omega_n = \pi T$ and $T=0.33$ of the approximate interaction [Eq. (1)] compared to the exact DCA interaction $\Gamma_{\text{even}}^{pp}$. $\phi(\mathbf{K}, \omega_n)$ has been normalized to its value at $\mathbf{K}=(\pi, 0)$.

pendence and the size of the d -wave eigenvalue are well accounted for by the simple form of the interaction given by Eq. (1). For the 4-site cluster, the eigenvalue λ_d is larger than that for the 24-site cluster because of the absence of pair field fluctuations for the 4-site cluster.¹⁴

In the following, we show the results for the 24-site cluster which was shown in Ref. 14 to be close to convergence with respect to the temperature dependence of the pair field susceptibility. The momentum dependence of the eigenfunction obtained using the approximate form of the interaction has the same dominant ($\cos K_x - \cos K_y$) behavior as the exact DCA result, as shown in Fig. 3. Furthermore, as shown in Fig. 4, the Matsubara frequency dependences of the DCA and the approximate interaction are remarkably similar.

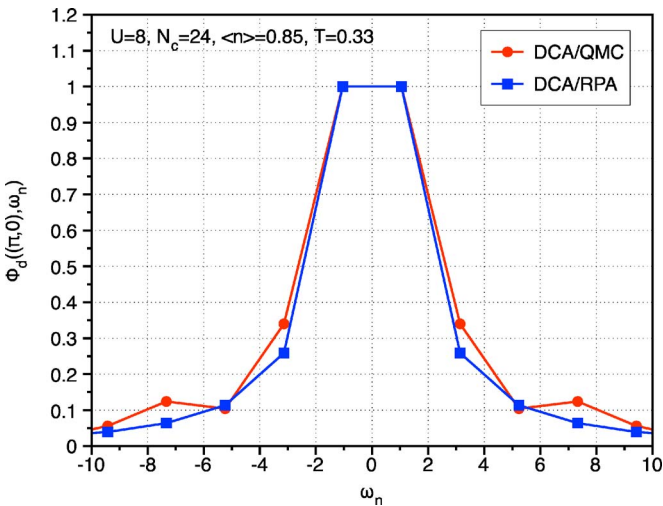


FIG. 4. (Color online) The frequency dependence of the d -wave eigenvector $\phi(\mathbf{K}, \omega_n)$ for $\mathbf{K}=(\pi, 0)$ and $T=0.33$ of the approximate interaction [Eq. (1)] compared to the exact DCA interaction $\Gamma_{\text{even}}^{pp}$. $\phi(\mathbf{K}, \omega_n)$ has been normalized to its value at $\omega_n = \pi T$.

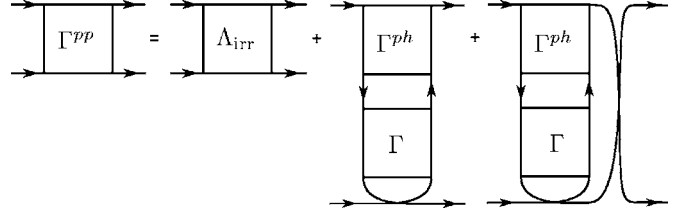


FIG. 5. Decomposition of the irreducible particle-particle vertex Γ^{pp} into a fully irreducible vertex Λ_{irr} plus reducible particle-hole contributions in the cross channel. Here, Γ denotes the full two-particle vertex and Γ^{ph} the irreducible particle-hole vertex.

IV. EFFECTIVE $\bar{U}(T)$

By fitting $\bar{U}(T)$ so that the d -wave strength of the approximate interaction is equal to that of the exact DCA interaction, we have found that the approximate form [Eq. (1)], does an excellent job in describing the d -wave eigenvalue and eigenfunction. From a purely phenomenological point of view, this is an important result. It means that to the extent that the Hubbard model gives an appropriate description of the cuprates, inelastic neutron-scattering experiments which give $\Im m \chi(q, \omega)$ provide a way of determining the momentum and frequency structure of the pairing interaction. A similar analysis was applied to the heavy fermion superconductor UPT₃.^{15,16}

One would like to have a better understanding of \bar{U} . As previously discussed in Refs. 17 and 18 and more recently in Refs. 1 and 2, the irreducible particle-particle vertex can be decomposed into a fully irreducible two-fermion vertex Λ_{irr} plus contributions from particle-hole channels, as illustrated in Fig. 5. These particle-hole channels can be separated into density ($S=0$) and magnetic ($S=1$) channels. For the even frequency, even momentum part of Γ^{pp} that is of interest, one has

$$\Gamma_{\text{even}}^{pp}(K, K') = \Lambda_{\text{irr,even}}(K, K') + \frac{1}{2}\Phi_d(K, K') + \frac{3}{2}\Phi_m(K, K') \quad (9)$$

with the even frequency, even momentum part of the fully irreducible two-particle vertex $\Lambda_{\text{irr,even}}$ and

$$\begin{aligned} \Phi_{dm}(K, K') &= \frac{1}{2} [\Gamma_{dm}^{red}(\mathbf{K} - \mathbf{K}', \omega_n - \omega_{n'}; \mathbf{K}', \omega_{n'}; -\mathbf{K}, -\omega_n) \\ &+ \Gamma_{dm}^{red}(\mathbf{K} + \mathbf{K}', \omega_n - \omega_{n'}; -\mathbf{K}', \omega_{n'}; -\mathbf{K}, -\omega_n) \\ &+ \Gamma_{dm}^{red}(\mathbf{K} - \mathbf{K}', \omega_n + \omega_{n'}; \mathbf{K}', -\omega_{n'}; -\mathbf{K}, -\omega_n) \\ &+ \Gamma_{dm}^{red}(\mathbf{K} + \mathbf{K}', \omega_n + \omega_{n'}; -\mathbf{K}', -\omega_{n'}; -\mathbf{K}, -\omega_n)]. \end{aligned} \quad (10)$$

Here, $K=(\mathbf{K}, \omega_n)$ and Γ_{dm}^{red} are the two-particle reducible contributions to the full four-point vertex Γ_{dm} calculated in the $S=0$ (d) or $S=1$ (m) channel, i.e., $\Gamma_{dm}^{red}(Q; K; K') = \Gamma_{dm}(Q; K; K') - \Gamma_{dm}^{ph}(Q; K; K')$, where Γ_{dm}^{ph} is the irreducible vertex in the corresponding channel. The center of mass

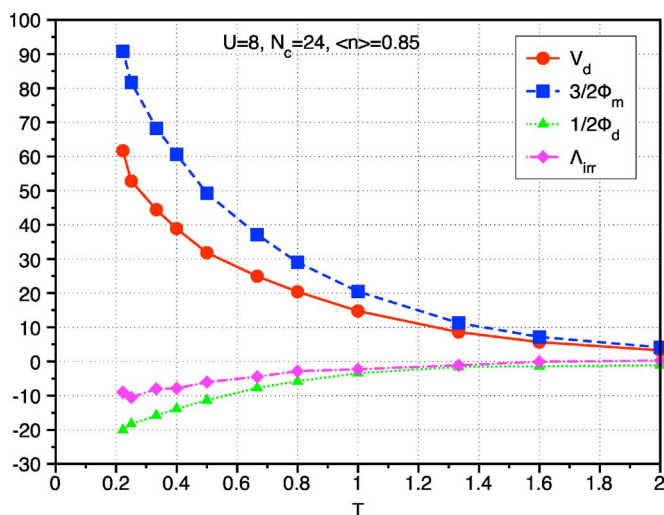


FIG. 6. (Color online) Decomposition of the d -wave pairing interaction V_d into d -wave projections of the fully irreducible vertex Λ_{irr} and a magnetic ($S=1$) channel $3/2\phi_m$ and a charge ($S=0$) channel $1/2\phi_d$.

and relative wave vectors and frequencies in these channels are labeled by the first, second, and third arguments, respectively. In Fig. 6, the d -wave projection [Eq. (6)] of $\Gamma_{\text{even}}^{pp}(K, K')$ along with the three contributions on the right-hand side of Eq. (9) is plotted versus the temperature. As expected, the dominant contribution comes from the magnetic ($S=1$) term. The fully irreducible channel is relatively ineffective, but at low temperatures, the charge density ($S=0$) channel acts to reduce the effective d -wave pairing strength. This is one of the reasons for the decrease found in $\bar{U}(T)$. A similar effect is found in the simple RPA treatment, where the effective pairing interaction is $V_{\text{spin}} - V_{\text{charge}}$. However, the RPA result for V_{charge} does not vary as strongly with the temperature.

In addition, from Fig. 5, one can see that even if one were to just consider the magnetic channel, \bar{U} would be a more complicated object. The coupling to the $S=1$ susceptibility is given by an irreducible particle-hole vertex $\bar{\Gamma}^{ph}$, which depends on $K-K'$ as well as on internal momenta and Matsubara frequencies. In Fig. 7, we show results for

$$\bar{\Gamma}^{ph} = \left(\frac{\langle g(\mathbf{K})\Phi_m(\mathbf{K}, \pi T; \mathbf{K}', \pi T)g(\mathbf{K}') \rangle_{\mathbf{K}\mathbf{K}'}}{\langle g(\mathbf{K})\chi_{\text{even}}(\mathbf{K}, \pi T; \mathbf{K}', \pi T)g(\mathbf{K}') \rangle_{\mathbf{K}\mathbf{K}'}} \right)^{1/2}, \quad (11)$$

where χ_{even} is the even frequency, even momentum part of the spin susceptibility χ obtained in an analogous manner to Eq. (7). One can see that this estimate for $\bar{\Gamma}^{ph}$ is smaller than

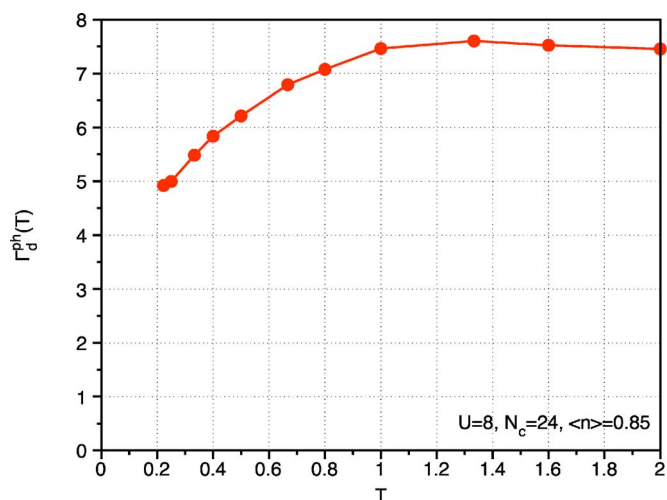


FIG. 7. (Color online) Coupling $\bar{\Gamma}^{ph}$ to the $S=1$ susceptibility calculated according to Eq. (11).

U . This is consistent with estimates for the spin effective interaction in a two-particle self-consistent approach^{19,20} and the results of earlier quantum Monte Carlo calculations^{21,22} which found that the electron-spin fluctuation vertex decreased with decreasing temperature for all momentum transfers.

V. CONCLUSION

To conclude, this work has shown that the momentum and frequency dependencies of the d -wave pairing interaction for the Hubbard model in the parameter regime which is believed to be appropriate to the cuprates are well approximated by the spin susceptibility. The strength of the coupling when written in the RPA form $\frac{3}{2}\bar{U}^2(T)$ requires a temperature-dependent effective $\bar{U}(T)$, which is reduced from the bare U and decreases at lower temperature in order to phenomenologically account for the effect of the charge channel and vertex corrections.

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