

Theory of spin and charge fluctuations in the Hubbard model

Y. M. Vil'k, Liang Chen, and A.-M. S. Tremblay

Département de Physique and Centre de Recherche en Physique du Solide, Université de Sherbrooke, Sherbrooke, Québec, Canada J1K 2R1

(Received 13 December 1993)

A self-consistent theory of both spin and charge fluctuations in the Hubbard model is presented. It is in quantitative agreement with Monte Carlo data at least up to intermediate coupling ($U \sim 8t$). It includes both short-wavelength quantum renormalization effects, and long-wavelength thermal fluctuations, which can destroy long-range order in two dimensions. This last effect leads to a small energy scale, as often observed in high-temperature superconductors. The theory is conserving, satisfies the Pauli principle, and includes three-particle correlations necessary to account for the incipient Mott transition.

The model introduced initially by Hubbard¹ for itinerant magnets is now widely used for high-temperature superconductors (HTSC) and other materials with strong interelectron interaction. Despite the apparent simplicity of the model, its properties remain poorly understood in the strongly to intermediate coupling regimes relevant for HTSC. Much experimental information on the magnetic fluctuations of these materials is now available from neutron scattering and nuclear magnetic resonance. A ubiquitous feature of the data is the presence of an unexplained small energy scale. The one-band Hubbard model near half-filling should contain this feature if it is the correct model for HTSC. Previous explanations^{2,3} of the magnetic correlations taking into account short-range quantum correlations (T -matrix effects) describe most of the Monte Carlo data except in the experimentally relevant regime. To our knowledge no explanation of the charge structure factor has appeared.

In this paper, we present a simple self-consistent approach to the two-dimensional (2D) Hubbard model that gives, without adjustable parameter, quantitative agreement with Monte Carlo data for spin and charge structure factors and susceptibilities at *all* fillings up to quite strong coupling. The approach takes into account not only the short-range quantum effects, but also the long-range thermal fluctuations that destroy antiferromagnetic long-range order in two dimensions at any finite temperature (Mermin-Wagner theorem). This is the key physical ingredient which leads to a small energy scale, and associated large correlation length, in the magnetic fluctuations. Previous approaches which included the long-range thermal fluctuations in the 2D Hubbard model were never applied to the incommensurate case relevant for HTSC. Furthermore, they are based on mode-coupling theory,⁴ which neglects charge fluctuations and does not include the effect of short-range quantum correlations, which are important not only for a quantitative description of the model but also for determining the nature of the ground state.

We first present our approach, discuss physical consequences, and finally compare with Monte Carlo data. We consider the one-band Hubbard model with on-site repulsive U . Our approach is motivated by the local field approximation, which was successful in the elec-

tron gas.⁵ We start from the equation of motion for the particle-hole operator $\rho_\sigma(\vec{l}, \vec{l}') = c_{\vec{l}, \sigma}^\dagger c_{\vec{l}', \sigma}$ in a weak external field $\phi_{\vec{l}, \sigma}$ which is coupled to the partial density operator $n_{\vec{l}, \sigma} = \rho_\sigma(\vec{l}, \vec{l}) = c_{\vec{l}, \sigma}^\dagger c_{\vec{l}, \sigma}$.⁶ After simple transformations, the term that contains the interaction in the equation of motion for $\rho_\sigma(\vec{l}, \vec{l}')$ is of the form

$$U[\langle \rho_\sigma(\vec{l}, \vec{l}') n_{\vec{l}, -\sigma} \rangle - \langle \rho_\sigma(\vec{l}, \vec{l}') n_{\vec{l}', -\sigma} \rangle]. \quad (1)$$

All operators contain the same time label, which is not explicitly written. The usual random phase approximation (RPA) corresponds to the neglect of two-particle correlations, namely one approximates $\langle \rho_\sigma(\vec{l}, \vec{l}') \rho_{-\sigma}(\vec{l}, \vec{l}') \rangle$ by $\langle \rho_\sigma(\vec{l}, \vec{l}') \rangle \langle \rho_{-\sigma}(\vec{l}, \vec{l}') \rangle$. This is clearly a poor approximation for on-site interactions because, as can be seen from (1), three of the four creation or annihilation operators in the correlator $\langle \rho_\sigma(\vec{l}, \vec{l}') \rho_{-\sigma}(\vec{l}, \vec{l}') \rangle$ are on the same lattice site \vec{l} . There is thus a strong correlation between two particle-hole pairs even when $|\vec{l} - \vec{l}'| \gg 1$ (the lattice constant is taken to be unity). We make use of this specific feature of the on-site interaction and neglect the dependence of the correlation coefficient on the lattice index l' which appears only once in the two-particle correlator. Mathematically, our ansatz is that the response of $\langle \rho_\sigma(\vec{l}, \vec{l}') n_{\vec{l}, -\sigma} \rangle$ to the external field ϕ is given by

$$\delta_\phi \langle \rho_\sigma(\vec{l}, \vec{l}') n_{\vec{l}, -\sigma} \rangle = \delta_\phi [g_{\uparrow\downarrow}(\vec{l}, \vec{l}') \langle \rho_\sigma(\vec{l}, \vec{l}') \rangle \langle n_{\vec{l}, -\sigma} \rangle], \quad (2)$$

where

$$g_{\sigma\sigma'}(\vec{l}, \vec{l}') = \frac{[\langle n_{\vec{l}, \sigma} n_{\vec{l}', \sigma'} \rangle - \langle n_{\vec{l}, \sigma} \rangle \langle n_{\vec{l}', \sigma'} \rangle]}{(\langle n_{\vec{l}, \sigma} \rangle \langle n_{\vec{l}', \sigma'} \rangle)} \quad (3)$$

is the pair correlation function between electrons of spin σ and σ' on the respective lattice sites \vec{l} and \vec{l}' .

It is important to realize that the pair correlation function in (1) and (2) cannot yet be taken equal to its equilibrium value $g_{\uparrow\downarrow}(\vec{l}, \vec{l}'; t) \neq g_{\uparrow\downarrow}(0)$ because of the weak external field $\phi_{\vec{l}, \sigma}$. In linear response the most general form for $g_{\uparrow\downarrow}(\vec{l}, \vec{l}'; t)$ is

$$g_{\uparrow\downarrow}(\vec{l}, \vec{l}'; t) = g_{\uparrow\downarrow}(0) + \sum_{l'} \int dt' \frac{\delta g_{\uparrow\downarrow}(\vec{l}, \vec{l}'; t)}{\delta \langle n_{\vec{l}', \uparrow}(t') \rangle} \delta \langle n_{\vec{l}', \uparrow}(t') \rangle,$$

where $n_{\vec{r}}(t) = n_{\vec{r},\uparrow}(t) + n_{\vec{r},\downarrow}(t)$ and we use that in the paramagnetic state

$$\frac{\delta g_{\uparrow\downarrow}(\vec{l}, \vec{l}; t)}{\delta \langle n_{\vec{r},\uparrow}(t') \rangle} = \frac{\delta g_{\uparrow\downarrow}(\vec{l}, \vec{l}; t)}{\delta \langle n_{\vec{r},\downarrow}(t') \rangle} \equiv g'_{\uparrow\downarrow}(\vec{l} - \vec{l}', t - t').$$

Note that the terms describing the response of $g_{\uparrow\downarrow}(\vec{l}, \vec{l}; t)$ to the external field enter the equation of motion only in a form that is symmetric in spin indices. Since the z component of spin $S_z = n_{\uparrow} - n_{\downarrow}$ is antisymmetric in n_{σ} and all equations are linear, it immediately follows that $g'_{\uparrow\downarrow}(\vec{l} - \vec{l}', t - t')$ enters the equation for charge but not for spin. This important simplification occurs because the Pauli principle precludes the appearance of terms like $\frac{\delta g_{\uparrow\uparrow}}{\delta \langle n_{\uparrow} \rangle} \neq \frac{\delta g_{\uparrow\uparrow}}{\delta \langle n_{\downarrow} \rangle}$ in the case of on-site interaction. After standard transformations (see, for example, Ref. 6) the spin and charge susceptibilities have the RPA form but with a renormalized effective interaction, which is different for spin (U_{sp}) and charge (U_{ch}):

$$U_{\text{sp}} = g_{\uparrow\downarrow}(0)U; \quad U_{\text{ch}} = [g_{\uparrow\downarrow}(0) + \delta g_{\uparrow\downarrow}(\omega, \vec{q})]U, \quad (4)$$

where $\delta g_{\uparrow\downarrow}(\omega, \vec{q}) = g'_{\uparrow\downarrow}(\omega, \vec{q}) \frac{n}{2}$, $g'_{\uparrow\downarrow}(\omega, \vec{q})$ is the Fourier transform of $g'_{\uparrow\downarrow}(\vec{l} - \vec{l}', t - t')$ and n is the band filling (half-filled case corresponds to $n = 1$). $\delta g_{\uparrow\downarrow}(\omega, \vec{q})$ is a three-particle correlation function, so that further simplification will be needed to calculate the charge susceptibility $\chi_{\text{ch}}(\omega, \vec{q})$. However, no further approximation is needed for the spin susceptibility $\chi_{\text{sp}}(\omega, \vec{q})$! Indeed, due to the Pauli principle, $g_{\uparrow\uparrow}(0) = 0$ so the spin part of the problem may be closed by using $g_{\uparrow\downarrow}(0) = -2g_{\text{sp}}(0)$ with $g_{\text{sp}}(l, l') \equiv [g_{\uparrow\uparrow}(l, l') - g_{\downarrow\downarrow}(l, l')]/2$ and the fluctuation-dissipation theorem (FDT) for spin:

$$g_{\text{sp}}(l, l') = \frac{1}{n} \int \frac{d^2 q}{(2\pi)^2} [S_{\text{sp}}(\vec{q}) - 1] e^{i\vec{q} \cdot (l - l')}, \quad (5)$$

$$S_{\text{sp}}(\vec{q}) = \frac{T}{n} \sum_{i\omega_m} \frac{\chi_0(i\omega_m, \vec{q})}{1 - (U_{\text{sp}}/2)\chi_0(i\omega_m, \vec{q})}.$$

The first equation is the definition of the spin structure factor; the second is a convenient form of the FDT with temperature T and bosonic Matsubara frequencies $i\omega_m$. The integral is over the first Brillouin zone. The definition of $\chi_0(i\omega_m, \vec{q})$ is the same as in Ref. 6.

For $\delta g_{\uparrow\downarrow}(\omega, \vec{q})$, we use the simplest ansatz, namely, that it is a constant $\delta g_{\uparrow\downarrow}$, which we determine self-consistently using the Pauli principle $g_{\uparrow\uparrow}(0) = 0$, the definition for the static charge structure factor

$$g_{\text{ch}}(l, l') = 1 + \frac{1}{n} \int \frac{d^2 q}{(2\pi)^2} [S_{\text{ch}}(\vec{q}) - 1] e^{i\vec{q} \cdot (l - l')}, \quad (6)$$

and the FDT for charge. We thus have a simple theory with only two parameters $g_{\uparrow\downarrow}(0)$ and $\delta g_{\uparrow\downarrow}$ that are found self-consistently. It can be explicitly checked that charge, spin, and energy are conserved. As with all self-consistent theories, the usefulness of the approach can be judged only *a posteriori* by comparison with numerical or exact results. We provide such comparisons later in the paper.

The absence of a magnetic phase transition at any finite temperature in 2D follows immediately from the

above approach. Define the mean-field critical value of U by $U_{mf,c} = 2/\chi_0(0, \vec{q}_{\text{max}})$, where $\chi_0(i\omega_m, \vec{q}_{\text{max}})$ is the susceptibility of noninteracting electrons and \vec{q}_{max} is the value of \vec{q} at which the static susceptibility has its maximum. If $U_{\text{sp}} = g_{\uparrow\downarrow}(0)U$ in (5) was large enough for the transition to occur, namely $\delta U = [U_{mf,c} - g_{\uparrow\downarrow}(0)U] = 0$, then the \vec{q} integral for the static susceptibility ($\omega_m = 0$) in the expression for $g_{\text{sp}}(0)$ [Eq. (5)] would diverge logarithmically so that $g_{\uparrow\downarrow}(0) = -2g_{\text{sp}}(0)$ would become negative, in obvious contradiction with $\delta U = 0$. Hence, in our approach, magnetic fluctuations always push the value of $g_{\uparrow\downarrow}(0)$ away from its critical value $g_{\uparrow\downarrow}^{(c)}(0) = U_{mf,c}/U$ at any finite temperature. Furthermore, for a wide range of values of $U > U_{mf,c}$ and $T < T_{mf,c}$, the system will be quite close to magnetic instability ($\delta U \sim 0$), providing the basis for a generic explanation of the small energy scale observed in HTSC. In the regime in which the temperature is larger than this small energy scale, the correlation length grows exponentially $\xi \propto \xi_0 e^{\text{const}/T}$ ($\xi^{-2} \equiv \delta U/U_{mf,c}$), reflecting the logarithmic divergence mentioned above. This is typical behavior for systems at their lower critical dimension. When a real quasi-two-dimensional system enters this regime, small three-dimensional effects can easily stabilize long-range order.

We digress briefly to speculate on how the phase diagram of a system with weak three-dimensional effects would then look. We neglect effects, such as disorder, which may become important when the small energy scale δU appears. We define a quasicritical temperature T_{qc} as the temperature at which the enhancement of the magnetic susceptibility $\tilde{\xi}^2 = \chi_{\text{sp}}(0, \vec{q}_{\text{max}})/\chi_0(0, \vec{q}_{\text{max}})$ is of order 500. Calculations for the nearest-neighbor Hubbard model show that $\tilde{\xi}^2$ increases by an order of magnitude when the temperature is reduced below T_{qc} by as little as $T_{\text{qc}} - T \sim 0.01$ (all energies are in units of the hopping integral t). In our theory, the emerging long-range order is determined by the position of the maximum of $\chi_0(0, \vec{q})$. At $T = 0$, as soon as $n \neq 1$, two-dimensional Fermi-surface effects⁸ lead to a maximum with a cusplike singularity in the $(\pi, \pi) - (\pi, 0)$ direction. The situation is different at finite temperature where the maximum can be at $\vec{q}_{\text{max}} = (\pi, \pi)$ even for $n < 1$. Figure 1 shows a rough magnetic phase diagram obtained by approximating T_c by T_{qc} (with $U = 2.5$). The insets show the dependence of $q_{y,\text{max}}$ [$\vec{q}_{\text{max}} = (\pi, q_{y,\text{max}})$] and of the enhancement factor $\tilde{\xi}^2$ on temperature for three different fillings. The filling $n = 0.93$ is marginal in the sense that the shift of \vec{q}_{max} from (π, π) occurs when the enhancement $\tilde{\xi}^2$ is already quite large. We would expect then that long-range order would be antiferromagnetic for $n > 0.93$ and incommensurate spin-density wave for $0.89 < n < 0.93$.

Let us now discuss the limit $T \rightarrow 0$. In Fig. 2, we show the renormalized spin interaction U_{sp} as a function of the filling n for $U = 2.5$ and $U \rightarrow \infty$, together with $U_{mf,c}(n)$. Remarkably, at low filling the value of U_{sp} saturates to $U_{\text{sp}} \approx 3.2$ as the bare interaction increases $U \rightarrow \infty$. This quantum effect was anticipated by Kanamori,^{7,2} who argued that the largest value of U_{sp} is proportional to the kinetic energy cost to put a node in

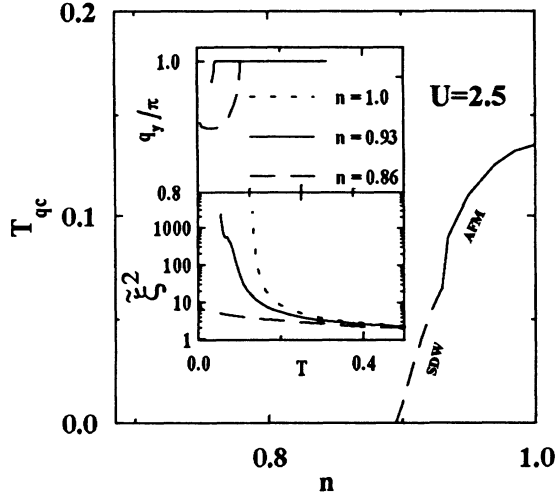


FIG. 1. Approximate phase diagram of the quasi-2D Hubbard model with T_c approximated by T_{qc} . The inset shows the temperature dependence of $q_{\max}(T)$ and the enhancement factor $\xi^2 = \chi_{sp}(0, q_{\max})/\chi_0(0, q_{\max})$ for three different fillings n .

the two-body wave function where two electrons overlap. At a sufficiently large filling, when $U_{sp}(n)$ starts to follow $U_{mf,c}(n)$ for $T \rightarrow 0$, the paramagnetic state has an instability at exactly $T = 0$. The existence of an upper limit for U_{sp} leads to the existence of a lower limit for the filling $n_{c,\min} \approx 0.685$ below which there is no magnetic phase transition at any U . This, in turn, means that only spin-density waves with $\vec{q} = (\pi, q_y)$, $q_y/\pi \in [0.74, 1]$ are possible. In particular, the ferromagnetic state does not exist in the Hubbard model on a square lattice² and there is also a temperature $T \approx 0.5$ above which there is no exponential regime for $\xi(T)$ at any U where our theory applies.

In the rest of this paper, we compare our theoretical results for infinite lattice with Monte Carlo simulations. Finite-size effects are expected to become important in simulations when the correlation length becomes comparable with system size. The largest size effects

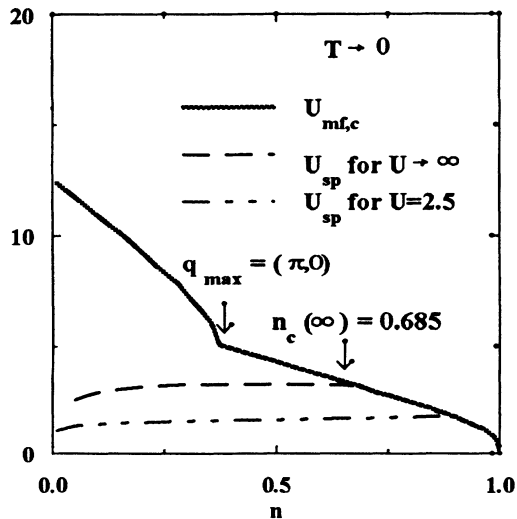


FIG. 2. Filling dependence of U_{sp} and $U_{mf,c}$ as $T \rightarrow 0$.

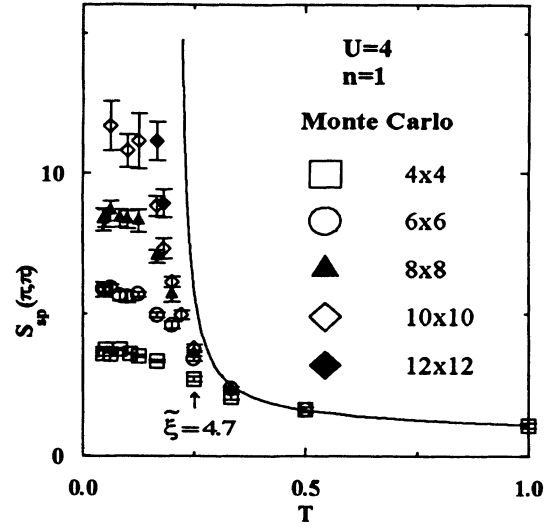


FIG. 3. Temperature dependence of $S_{sp}(\pi, \pi)$ at half-filling $n = 1$. The solid line is our theory; symbols are Monte Carlo data from Ref. 9.

are thus expected in $S_{sp}(\pi, \pi)$ at half-filling ($n = 1$). This is shown in Fig. 3. The Monte Carlo data⁹ follow our theoretical curve (solid line) until they saturate to a size-dependent value. We checked that finite-size effects for $S_{sp}(\vec{q})$ away from the antiferromagnetic wave vector $\vec{q} = (\pi, \pi)$ are much smaller, so that, even for 8×8 systems, theory and simulations agree very well for all other values of \vec{q} (not shown). Finite-size effects in the spin structure factor $S_{sp}(\vec{q})$ are not too important away from half-filling for the parameters shown in Figs. 4(a)–4(d). Obviously though, finite-size simulations cannot reproduce the small incommensurability captured by our theory at $n = 0.8$ in Fig. 4(d).

Figures 4(b) and 4(c) show that, even for relatively

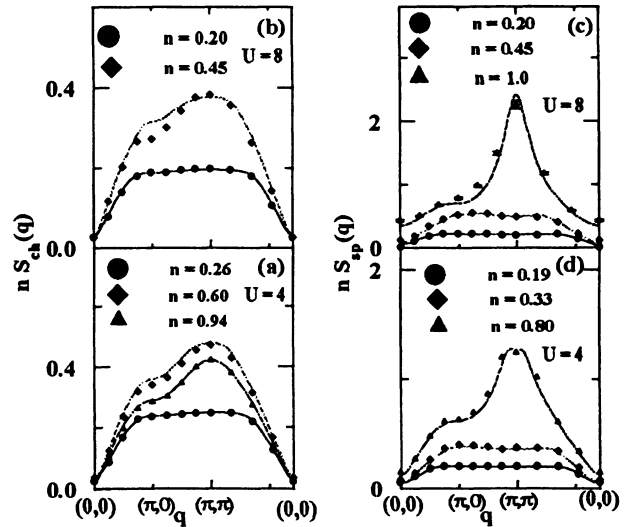


FIG. 4. Wave vector (\vec{q}) dependence of the spin and charge structure factors for different sets of parameters. Solid lines are our theory; symbols are our Monte Carlo data. Monte Carlo data for $n = 1$ and $U = 8$ are for 6×6 clusters and $T = 0.5$; all other data are for 8×8 clusters and $T = 0.2$. Error bars are shown only when significant.

strong coupling ($U \sim 8$), the theory agrees very well with *both* spin $S_{\text{sp}}(\vec{q})$ and charge $S_{\text{ch}}(\vec{q})$ structure factors. However the theory should eventually break down for $U \rightarrow \infty$. This can be seen in the half-filled case from the fact that, for $U \rightarrow \infty$, the antiferromagnetic susceptibility remains constant in our theory while mapping to the Heisenberg model with $J = 4t^2/U$ shows that it should decrease with U . It seems, however, that large- U asymptotic is reached for values of U much larger than the bandwidth.

Figure 4(a) shows that our theory reproduces the important qualitative fact that the charge structure factor $S_{\text{ch}}(\vec{q}; n)$ depends on filling in a nonmonotonous manner. The decrease of $S_{\text{ch}}(\vec{q})$ towards half-filling is a signature of the incipient Mott transition. The effect can be seen because our approach takes into account both three-particle correlations and the Pauli principle. Writing the Pauli principle as a sum-rule $\Sigma_{\vec{q}}[S_{\text{ch}}(\vec{q}) + S_{\text{sp}}(\vec{q})] = 2 \Sigma_{\vec{q}} S_0(\vec{q})$, the parameter $\delta g_{\uparrow\downarrow}$, which partially takes into account three-particle correlations, must increase close to half-filling in order to reduce $S_{\text{ch}}(\vec{q})$ and compensate for the increase in the contribution of the spin structure factor.

Our theory also explains the good fit of the dynamical spin susceptibility $\chi_{\text{sp}}(i\omega_m, \vec{q})$ obtained by Bulut, Scalapino, and White³ using RPA with $U_{\text{ren}} = 2$. Indeed, for $U = 4$, $n \approx 0.87$ on 8×8 clusters, our calculations give $U_{\text{sp}} = 2.05$ with very little dependence on temperature. Bulut, Scalapino, and White³ have also shown that their Monte Carlo data for the self-energy $\Sigma(i\omega_m, \vec{q})$ can

be reasonably well fitted by the Berk-Schrieffer formula¹⁰ with the same $U_{\text{ren}} = 2$. In our approach, the expression for $\Sigma(i\omega_m, \vec{q})$ in terms of susceptibilities should come at the next level of approximation. Bulut *et al.*¹¹ have also fitted a number of experiments in HTSC by fine tuning the value of U_{ren} close to a magnetic instability ($\delta U \sim 0$). In our approach, a wide range of bare values of U naturally renormalizes to such a situation.

In conclusion, imposing the Pauli principle as well as self-consistency through the fluctuation-dissipation theorem, we have formulated a simple theory that also satisfies conservation laws and gives, without adjustable parameter, a quantitative explanation of Monte Carlo data for both spin and charge structure factors as well as susceptibilities up to intermediate coupling. Both short-wavelength quantum renormalization effects and long-wavelength thermal fluctuation effects, which destroy long-range order in two dimensions, are accounted for. The latter effect naturally leads to a small energy scale for a wide range of parameters, possibly giving a microscopic origin for the small energy scale observed in experiments on high-temperature superconductors.

We thank A.E. Ruckenstein for useful discussions. This work was partially supported by the Natural Sciences and Engineering Research Council of Canada (NSERC), the Fonds pour la formation de chercheurs et l'aide à la recherche from the Government of Québec (FCAR), (A.-M.S.T.) the Canadian Institute of Advanced Research (CIAR), and the Killam foundation.

¹ J. Hubbard, Proc. R. Soc. London A **276**, 238 (1963).

² L. Chen, C. Bourbonnais, T. Li, and A.-M. S. Tremblay, Phys. Rev. Lett **66**, 369 (1991).

³ N. Bulut, D. J. Scalapino, and S. R. White, Phys. Rev. B **47**, 2742 (1993).

⁴ For a review, see T. Moriya, *Spin Fluctuations in Itinerant Electron Magnetism* (Springer-Verlag, Berlin, 1985).

⁵ For a review, see K. S. Singwi and M. P. Tosi, in *Solid State Physics*, edited by H. Ehrenreich, F. Seitz, and D. Turnbull (Academic, New York, 1981), Vol. 36, p. 177; S. Ichimaru, Rev. Mod. Phys. **54**, 1017 (1982).

⁶ D. Pines and P. Nozières, *Theory of Quantum Liquids* (Ben-

jamin, New York, 1966), Vol. I.

⁷ J. Kanamori, Prog. Theor. Phys. **30**, 275 (1963).

⁸ P. Bénard, L. Chen, and A.-M. S. Tremblay, Phys. Rev. B **47**, 15217 (1993); J. P. Lu, Q. Si, J. H. Kim, and K. Levin, Phys. Rev. Lett. **65**, 2466 (1990).

⁹ S. R. White, D.J. Scalapino, R. L. Sugar, E. Y. Loh, Jr., J. E. Gubernatis, and R. T. Scalettar, Phys. Rev. B **40**, 506 (1989).

¹⁰ N. F. Berk and J. R. Schrieffer, Phys. Rev. Lett. **17**, 433 (1966).

¹¹ N. Bulut, D. Hone, D. J. Scalapino, and N. E. Bickers, Phys. Rev. Lett. **64**, 2723 (1990).