Magnetic Properties of the Two-Dimensional Hubbard Model

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Monte Carlo simulations of the magnetic structure factor of the two-dimensional Hubbard model are in qualitative agreement with the slave-boson approach and, in the low-temperature intermediate-coupling limit, they are in even better quantitative agreement with the random-phase approximation, as long as a renormalized repulsion U is used. This renormalization comes from maximally crossed diagrams, which account for two-body short-range correlations. One of the consequences is that Stoner ferromagnetism is not a generic property of the two-dimensional one-band Hubbard model.

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In 1963, Kanamori[1] introduced in the study of itinerant ferromagnetism an important concept which he drew from Brueckner's theory[2] of nuclear matter and He. The model Kanamori was studying became later known as the Hubbard model.[3] The concept which he introduced is that "The importance of intra-atomic interaction . . . depends critically on how, and to what extent . . . Coulomb self-energy is reduced by the electron correlation. We calculate this reduction by taking into account the multiple scattering between two electrons." Kanamori argued that his calculation of these electron correlations was justified in the dilute limit,[4] and he went on to show that there was a critical electron concentration below which band ferromagnetism was impossible because the renormalized (effective) Hubbard interaction U could never become large enough. The physical argument which he gave, and which is basically correct, is that "When the intra-atomic interaction is large, electrons will avoid entering into the same [site] by the sacrifice of the one-electron energy of the order of the bandwidth. Thus, this increase of the one-electron energy corresponds to the effective magnitude of the interaction."

In the present Letter, we show that our Monte Carlo simulations of the magnetic structure factor of the one-band Hubbard model on 8×8 lattices, for all band fillings and for all temperatures small compared with the Fermi energy, can be quantitatively explained, except very close to half filling, by replacing the Hubbard interaction U in the random-phase approximation (RPA) calculation[5] by the full T matrix. One of the consequences is that the critical value of concentration for ferromagnetism found by Kanamori should be moved so close to half filling in two dimensions that it competes with magnetic order driven by nesting.

In Figs. 1(a)–1(c), the magnetic structure factor of the two-dimensional Hubbard model obtained from Monte Carlo simulations for small, $\rho=0.36$, intermediate, $\rho=0.6$, and large, $\rho=0.94$, fillings are shown with statistical error bars ($\rho=1$ is half filling). The Monte Carlo method used is the so-called determinantal or Blankenbecler-Scalapino-Sugar-Hirsch (BSSH) approach.[6] Dashed lines in the figures are the results of a RPA calculation[5,7] performed for a discrete system of the same size (8×8), using the fluctuation-dissipation theorem,

$$\langle S^z_{\mathbf{q}} S^z_{-\mathbf{q}}\rangle = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \frac{1}{1-e^{-\beta\omega}} \mathrm{Im}\chi(\mathbf{q},\omega)\,, \qquad (1)$$

where S^z on site i is defined by $n_{i\uparrow}-n_{i\downarrow}$, $\chi(\mathbf{q},\omega)$ is the corresponding spin susceptibility, and β is the inverse temperature in units where the hopping integral t as well as Planck's and Boltzmann's constants are all equal to unity. In these plots, there is a single fitting parameter, namely, U_{rn} (see Ref. 8 for a similar approach). While trivial single-particle energy shifts are absorbed in the chemical potential, band narrowing and single-particle lifetime effects coming from self-energy corrections are neglected.[9] The fit is less satisfactory near half filling where mode-coupling effects[10,11] neglected in our approach are expected because of the incipient antiferromagnetism.

There are few other analytical calculations of the dynamical response functions of the Hubbard model, for arbitrary wave vector and filling. We also present here the first test of the newly developed spin-rotation-invariant slave-boson approach[12,13] which is known to reduce to Landau theory in the long-wavelength limit, to the Gutzwiller result in the static limit, and to some form of RPA at the Brillouin zone corner. The results[14] represented by solid lines in Fig. 1(b) give, without adjustable parameters, a qualitatively correct but quantitatively less satisfactory fit of the Monte Carlo data.

Coming back to the RPA approach, the value of the renormalized interaction U_{rn} is almost temperature independent and its U dependence can be obtained from the following simple formula:

$$U_{\mathrm{rn}} = U/(1+U\Lambda)\,, \qquad (2)$$

where the values of U_{rn} in Figs. 1(b) and 1(d) are both

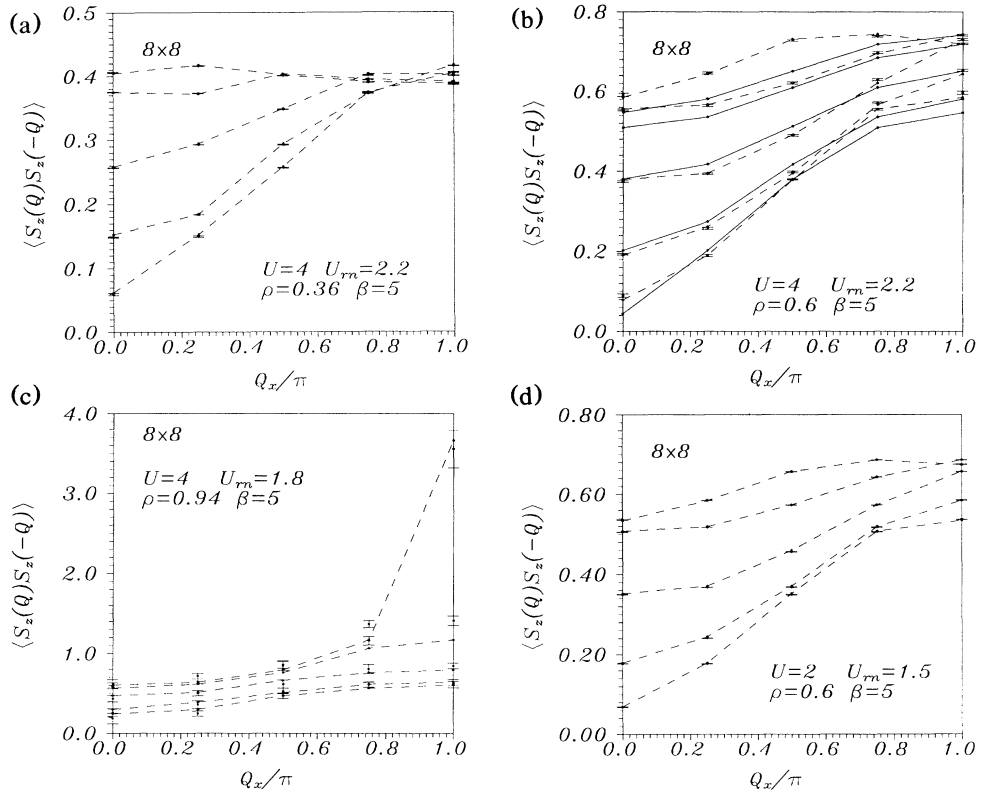

FIG. 1. Magnetic structure factor of the Hubbard model for 8×8 systems as a function of Q_x and Q_y. The dashed lines are obtained from RPA with a renormalized value $U_{\rm rn}$ of the interaction parameter U, in units where $t=1$. The bottom line is for $Q_y=0$ and the top one for $Q_y=\pi$, with a change of $\pi/4$ between every line. Monte Carlo results with $\Delta\tau=\frac{1}{8}$ are represented by error bars. (a)–(c) show various fillings, while (d) shows a different value of U for the same fillings as in (b). The solid lines in (b) are slave-boson results of Ref. 14 instead of RPA.

where the values of $U_{\rm rn}$ in Figs. 1(b) and 1(d) are both consistent with $\Lambda=0.2t^{-1}$ ($t=1$ in the figures). For U equal to the bandwidth $8t$ (not shown here) the RPA in conjunction with (2) starts to deviate from the Monte Carlo data[15] by about only 15%.

Equation (2) for the renormalized U is suggested by the vertex equation in the particle-particle channel

$$U_{\rm rn}(\mathbf{Q},iQ_n)=U-U\Lambda(\mathbf{Q},iQ_n)U_{\rm rn}(\mathbf{Q},iQ_n)\,, \tag{3}$$

where the kernel is

$$\Lambda(\mathbf{Q},iQ_n)=\frac{1}{N}\sum_{\mathbf{k}}\frac{[1-f(\varepsilon_{\mathbf{k}})][1-f(\varepsilon_{Q-\mathbf{k}})]-f(\varepsilon_{\mathbf{k}})f(\varepsilon_{\mathbf{Q}-\mathbf{k}})}{\varepsilon_{\mathbf{k}}+\varepsilon_{\mathbf{Q}-\mathbf{k}}-iQ_n}\,. \tag{4}$$

In this equation, $\varepsilon_{\mathbf{k}}=-2t(\cos k_x+\cos k_y)-\mu$, with μ the chemical potential, $f(\varepsilon_{\mathbf{k}})$ the Fermi function, N the number of sites, and iQ_n the Matsubara frequency which here plays the role that is played in a Schrödinger equation approach by the total energy of the incoming particles, measured with respect to the Fermi surface. The complete many-body calculation which includes this effect involves the solution of the coupled integral equations shown diagrammatically in Fig. 2. In the dilute limit and for hard-core interactions, one can justify the neglect of other classes of diagrams.[4,15] We have performed this calculation for the static $\mathbf{Q}=0$ susceptibility χ. The latter is related to the $\mathbf{Q}=0$ structure factor through the thermodynamic sum rule $\langle S^z_{\mathbf{Q}=0}S^z_{\mathbf{Q}=0}\rangle=T\chi$ which follows from the fluctuation-dissipation theorem for a conserved variable. We have checked that the solution of the equations in Fig. 2 does reproduce the Monte Carlo value of the $\mathbf{Q}=0$ magnetic structure factor as a function of filling. For $\rho=0.263$, $U=4$, $\beta=5$, for example, the diagrams give 0.037, while the Monte Carlo result is 0.038 ± 0.002. Between $\rho=0$ and $\rho=0.8$, the worst disagreement is 30% at $\rho=0.5$. The diagrams in Fig. 2 clearly show that the renormalized $U_{\rm rn}$ comes from maximally crossed diagrams. Physically, these diagrams take into account the fact that the two-body wave

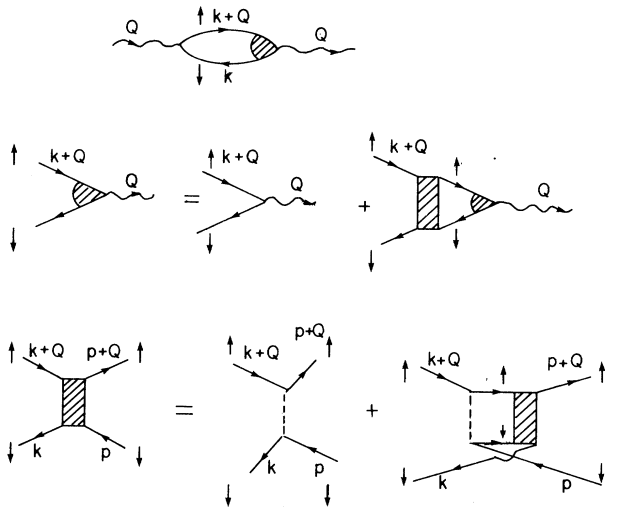

FIG. 2. Feynman diagrams which lead to the renormalized U. The calculation is for the $Q=0$ structure factor (static susceptibility). The S^+S^- susceptibility is on the first line. The vertex in the second line obeys the usual RPA equation except that the $\mathbf{Q},iQ_n$ dependence of the effective interaction in the last line is included. All external legs are shown only for labeling momenta and Matsubara frequencies.

function tends to vanish where the potential is large.

This calculation corroborates a simple approximation which consists in obtaining a value for $U_{\rm rn}$ by using in Eq. (2) the value of Λ in Eq. (4) and averaging the $\mathbf{Q}$ dependence over the Brillouin zone with the kernel Λ evaluated at $iQ_n=0$. That $iQ_n=0$ is a good approximation even when $\mathbf{Q}$ is different from zero probably comes from the fact that the Fermi factors of the Lindhard function force the particles at the entrance of the T matrix to be near the Fermi surface, corresponding on average to zero total energy. The averaging over $\mathbf{Q}$ is suggested by the fact that the sum of the momenta entering the particle-particle vertex in Fig. 2 can vary over a broad range, even when the particles are near the Fermi surface. The simple approximation just described predicts that $U_{\rm rn}$ decreases monotonously from 2.5 to 1.9 with increasing band filling when the bare U is equal to 4. This is within $\pm 15\%$ of the values found by fitting Monte Carlo data, namely, $U_{\rm rn}$ about equal to 2.2 until very close to half filling. It should also be clear that $U_{\rm rn}$ does not depend very much on details of the band structure or on temperature because it is an average over the Brillouin zone. We have checked that when the temperature scale is much less than the Fermi energy, the temperature dependence of $U_{\rm rn}$ can indeed by neglected, except close to half filling. That temperature dependence close to half filling ($\rho \gtrsim 0.8$) is another indication that mode-coupling effects[9,11,16] become important in that region and that our approach becomes less accurate.

Our results imply that to find magnetic instabilities of the paramagnetic phase with the RPA, the value of U which must be used should be $U_{\rm rn}$, which is smaller than the bare U extracted from experiments in the pure antiferromagnetic phase. This moves the paramagnetic to antiferromagnetic [or spiral, or spin-density-wave[17] (SDW)] phase boundary closer to half filling. The most striking modification of the RPA phase diagram brought about by our results is the complete disappearance of the Stoner ferromagnetic phase. On the basis of an approximation to (2) and (4), Kanamori[1] had suggested earlier the disappearance of Stoner ferromagnetism at very low band filling but, in fact, this conclusion extends to all concentrations. Indeed, the largest possible value of $U_{\rm rn}$, namely, the Brillouin-zone average of $1/\Lambda$, is of the order of the bandwidth and not large enough to lead to ferromagnetism at low concentration; and near half filling the RPA Stoner criterion for the simplest cosine band in two dimensions leads instead to finite-wave-vector instabilities.[17] Band ferromagnetism,[18] if it occurs, does so only for values of U which are very much larger than the bandwidth, outside the range of validity of RPA. The slave-boson approach[12] predicts ferromagnetism for values of U larger then about $120t$, and a Kanamori limit of about $\rho=0.62$, closer to half filling than found by Kanamori. However, the physics of ferromagnetism in the very-large-U limit is that of Nagaoka,[19] which consists in minimizing kinetic energy with no double occupancy, and hence is quite different from that of Stoner which involves a compromise between kinetic and potential energy.

Assuming that our simple approximate way of estimating $U_{\rm rn}$ holds in three and four dimensions as well, we find that the Stoner criterion can almost be fulfilled near the maximum of the density of states. The uncertainties of our estimate for the maximum value of $U_{\rm rn}$ do not allow us then to completely exclude ferromagnetism.[20] However, the absence of Stoner ferromagnetism also in infinite dimension[21] suggests that the Stoner model of ferromagnetism is not generic[18] in any dimension. Only band structures with peaks in the density of states and no concomitant nesting wave vector could lead to Stoner ferromagnetism.

In conclusion, our detailed comparisons with Monte Carlo calculations show how a simple RPA approach with renormalized U can accurately describe the magnetic properties of the Hubbard model in the weak- to intermediate-coupling limit for almost the whole range of band fillings and temperatures. The only exception is very close to half filling where a single temperature-independent value of $U_{\rm rn}$ does not fit all wave vectors. The RPA approach has recently been used to understand various aspects of the Hubbard model.[17,22] By contrast, slave-boson approaches[12-14] seem also qualitatively correct but are less accurate in this intermediate-coupling limit. We are left with the hope that they give a reasonable phase diagram in the very-large-U limit.

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