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1997 J. Phys.: Condens. Matter 9 L267

(http://iopscience.iop.org/0953-8984/9/18/003)

J. Phys.: Condens. Matter **9** (1997) L267–L273. Printed in the UK PII: S0953-8984(97)79402-5

**LETTER TO THE EDITOR**

# Frequency-dependent spin susceptibility in the two-dimensional Hubbard model

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Received 5 February 1997

**Abstract.** A quantum Monte Carlo calculation of the dynamical spin susceptibility in the half-filled 2D Hubbard model is presented for temperature $T = 0.2t$ and an intermediate on-site repulsion $U = 4t$. Using the singular-value decomposition technique we succeed in analytically continuing the Matsubara Green's function into the real-frequency domain and in deriving the spectral representation for longitudinal and transverse spin susceptibility. The simulation results, while contradicting the random-phase approximation prediction of antiferromagnetic long-range order at this temperature, are in agreement with an extension of the self-consistent renormalization approach of Moriya. The static susceptibility calculated using this technique is qualitatively consistent with the $\omega \to 0$ simulation results.

The dynamical magnetic susceptibility in strongly correlated electron systems (SCES) has been at the centre of attempts to explain the pairing mechanism in high-temperature superconductivity (HTSC) [1, 2] as well as to understand the normal-state properties of the HTSC compounds [3, 4]. The frequency dependence of the magnetic susceptibility can be measured in neutron scattering experiments, thus allowing the assessment of the relevance of various low-energy models of SCES to HTSC, and the validity of their approximate solutions over a range of temperatures and dopings. Quantum Monte Carlo (QMC) simulations, among other numerical techniques, provide an alternative test of these models and of the applicability of the analytical approximations. These simulations supply direct information only about the imaginary-time dependence of the correlation functions. Therefore, most of the information derived from them has been concerned with the static susceptibility [5, 6]. Analytic continuation of QMC data into the real-time domain has been performed recently to obtain the single-particle spectral weight function [7, 8] and two-particle [9] Green's functions. However, a comprehensive dynamical description of the SCES, particularly of their collective excitations, based on QMC simulations, remains a largely unexplored area. In this letter we report results of analytic continuation by means of singular-value decomposition (SVD) to evaluate the dynamical spin susceptibility. These results allow us to examine spectral characteristics predicted in the spin-density-wave (SDW) treatment [1] for a 2D Hubbard model at finite temperature.

Interpretations of QMC results for magnetic susceptibility have been mostly related to random-phase-approximation (RPA) calculations which lead to an SDW ground state [1]. Comparisons have been made between finite-lattice simulations and RPA results for an infinite system [5, 10]. RPA calculations however overestimate the value of the Néel temperature [6, 11] which would only be enhanced in a calculation done on a finite lattice [12]. Even without this enhancement, the fit of the QMC data to the RPA prediction requires an artificial correction to the bare Coulomb repulsion in the RPA expression for the

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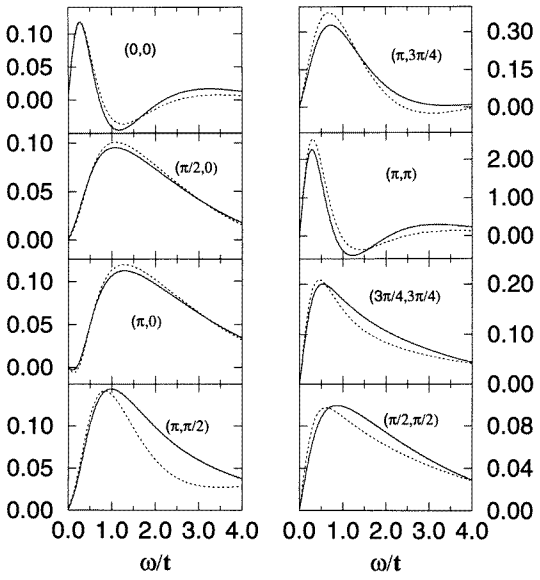


**Figure 1.** $\frac{1}{2}\chi''^{zz}(\boldsymbol{k},\omega)$ (solid line) and $\chi''^{+-}(\boldsymbol{k},\omega)$ (dotted line) versus $\omega$ for selected values of the lattice momentum, given in the brackets in each figure. $\chi''^{zz}$ is divided by 2 to make the comparison easier.

susceptibility [5, 12, 13]. We explored, therefore, an application of an extended version of the self-consistent-renormalization (SCR) theory which is known to provide a more accurate description of weak antiferromagnetism [11], and found that for a finite system this theory agrees qualitatively with the QMC results with no parameter adjustment.

We apply a finite-temperature QMC algorithm simulating the partition function of the Hubbard model as a path integral of a euclidean field theory. The temperature is represented by an additional compact dimension whose extent is equal to the inverse temperature $\beta$. Matsubara Green's functions $G_{S_1S_2}(\tau)$ for the spin operators $S_1$ and $S_2$, satisfying, for imaginary-time separation $\tau$, $G(\tau+\beta)=G(\tau)$, are evaluated as ensemble averages of the type

$$G_{S_1S_2}(\tau)=\frac{\mathrm{Tr}\left[\mathrm{e}^{\tau H}S_1\mathrm{e}^{-\tau H}S_2\mathrm{e}^{-\beta H}\right]}{\mathrm{Tr}\,\mathrm{e}^{-\beta H}} \qquad (0<\tau\leqslant\beta) \tag{1}$$

where $H$ is the Hamiltonian of the system and the trace is taken over all of the degrees of freedom. Analytic continuation of these functions into real time amounts to a solution of the following ill-posed inverse problem:

$$G(\tau)=\int_{-\infty}^{\infty}\mathrm{d}\omega\,\frac{\mathrm{e}^{-\omega\tau}}{1-\mathrm{e}^{-\omega\beta}}\,\chi''(\omega) \qquad (0<\tau\leqslant\beta). \tag{2}$$

$\chi''(\omega)$ is the imaginary part of the Fourier image of the commutator retarded Green's function. The solution for $\chi''(\omega)$ was found using the singular-value decomposition technique described in reference [8].

We calculate spin-correlation functions derived from QMC simulation data for Matsubara Green's functions of the type

$$\begin{aligned} G_{S^zS^z}(\boldsymbol{k},\tau)&=\langle(n_\uparrow(\boldsymbol{k},\tau)-n_\downarrow(\boldsymbol{k},\tau))(n_\uparrow(-\boldsymbol{k},0)-n_\downarrow(-\boldsymbol{k},0))\rangle \\ G_{S^+S^-}(\boldsymbol{k},\tau)&=\langle c_\uparrow^\dagger(\boldsymbol{k},\tau)c_\downarrow(\boldsymbol{k},\tau)\,c_\downarrow^\dagger(-\boldsymbol{k},0)c_\uparrow(-\boldsymbol{k},0)\rangle \end{aligned} \tag{3}$$

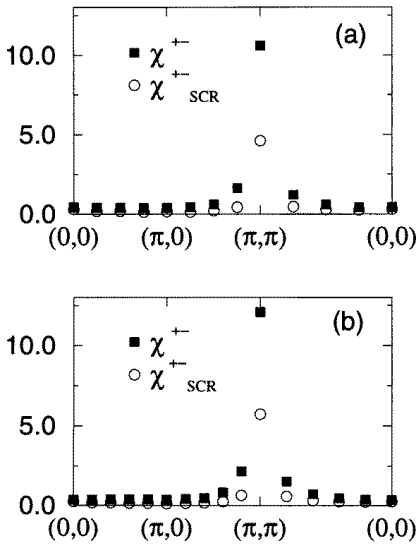


**Figure 2.** The static spin susceptibility versus the lattice momentum; (a) an $8^2$ lattice, (b) a $10^2$ lattice. The results of the SCR calculation are shown by ○.

where $c_\sigma^\dagger$ ($c_\sigma$) is an electron creation (annihilation) operator with spin projection $\sigma$, $n_\sigma = c_\sigma^\dagger c_\sigma$, and $\boldsymbol{k}$ is the lattice momentum. The simulations were performed for a single-band 2D Hubbard model with on-site Coulomb repulsion $U = 4t$ ($t$ being the nearest-neighbour hopping parameter) at a simulation temperature $1/\beta = 0.2t$, and for lattice sizes $8^2$ and $10^2$. The models were simulated at half-filling. We solve equation (2) with its left-hand side given by $G_{S^zS^z}(\boldsymbol{k}, \tau)$ and $G_{S^+S^-}(\boldsymbol{k}, \tau)$, the solutions $\chi''(\boldsymbol{k}, \omega)$ being the imaginary parts of the dynamical longitudinal ($\chi^{zz}(\boldsymbol{k}, \omega)$) and transverse ($\chi^{+-}(\boldsymbol{k}, \omega)$) susceptibilities respectively.

We found that the simulation results were sensitive to the discretization of the imaginary-time axis $\delta\tau$. To achieve stable results it was necessary to reduce the spacing to a level of $U\,\delta\tau = 0.25$. In figure 1 we present the results for $\chi''(\boldsymbol{k}, \omega)$ for various values of the lattice momentum $\boldsymbol{k}$. The data are based on up to 6700 measurements on an $8^2$ lattice. The ensemble averages and the statistical errors were estimated using bootstrap analysis. The analytic continuation has been based on reconstruction with up to seven singular functions of the kernel in equation (2), which corresponds to the number of singular values whose ratio to the largest one is larger than the average error ($\mathcal{O}(10^{-2})$). The Matsubara Green's functions were evaluated accordingly at seven values of $\tau$, their spacing corresponding to the zeros of the seventh singular vector. The negative side-lobes in the reconstructed function are due to the limited singular-function bandwidth. As was pointed out in reference [8], their appearance is similar to that of Airy rings with negative side-lobes which result from imaging a positive $\delta$-function over a limited Fourier bandwidth.

A sum rule used in reference [14] for the $t$–$J$ model can be applied in our case to examine the extent of double occupancy in the given temperature and coupling regime. With our normalization (see equation (2)), this sum rule reads

$$\frac{1}{N}\int_0^\infty \mathrm{d}\omega \sum_{\boldsymbol{k}} \coth\frac{\beta\omega}{2}\chi''^{zz}(\boldsymbol{k}, \omega) = \left\langle (S_i^z)^2 \right\rangle \tag{4}$$

where $N$ is the number of lattice sites. The r.h.s. of this equation was obtained directly from the simulation data of the $\tau = 0$ spin correlations, and the l.h.s. was obtained from analytic continuation of the Matsubara Green's functions. The agreement between these two

constitutes a consistency check on the analytic continuation. The two calculations do indeed agree, and give $\langle (S_i^z)^2 \rangle \approx 0.74$, which suggests that 13% of the sites are doubly occupied. This significantly violates the constraint assumed in the $t$–$J$ model, and undermines the validity of extrapolating results derived for the $t$–$J$ model to the Hubbard model in this regime of coupling and temperature [15].

To compare our results with those derived from the SDW-RPA treatment, we examine our results with respect to the evidence for long-range antiferromagnetic ordering. The SDW-RPA treatment predicts, for the size of systems simulated, a Néel temperature $T_{\text{Néel}}^{\text{RPA}} \approx 0.7t$, which is above our simulation temperature. The same treatment predicts also an SDW gap $\Delta = 1.38t$ at our simulation temperature. This gap would result in the vanishing of the time-ordered Green's function, $\chi''^{zz\,T}(\boldsymbol{Q}, \omega)$, at the nesting vector $\boldsymbol{Q} = (\pi, \pi)$ for $\omega < 2\Delta$ [1].

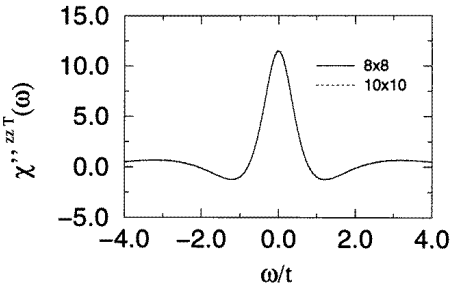


**Figure 3.** The time-ordered Green's function $\chi''^{zz\,T}(\boldsymbol{Q}, \omega)$. Note the absence of an SDW gap.

We find that $\chi''(\boldsymbol{k}, \omega)$ for small values of $\omega$ has a clear peak at $\boldsymbol{k} = \boldsymbol{Q}$, which leads also to a sharply enhanced real part of the static susceptibility $\chi'(\boldsymbol{Q}, \omega = 0)$ calculated using the Kramers–Kronig relations (figure 2). However, our results contradict two essential SDW predictions: the spontaneous breaking of rotational symmetry and the existence of a gap in the spectral function for the magnetic correlations. The ratio of 2 between the longitudinal and transverse susceptibilities, which is particularly accurate for local correlation functions and is maintained for $\chi^{zz}(\boldsymbol{k}, \omega)$ and $\chi^{+-}(\boldsymbol{k}, \omega)$ (figure 1), indicates that the rotational symmetry is not violated, while the results for $\chi''^{zz\,T}(\boldsymbol{Q}, \omega)$ (figure 3) show no evidence for the SDW gap. The persistence of this latter discrepancy with the SDW prediction was examined for increase of the lattice size to $10^2$ (results for the two lattices are superimposed in figure 3). Since the sign of the gap is invariant under the change of the staggered magnetization, if antiferromagnetic order existed in the thermodynamical limit we would expect a minimum (if not vanishing) of $\chi''^{zz\,T}(\boldsymbol{Q}, \omega)$ for small values of $\omega$. This is clearly absent in our results.

We observe therefore that our results cannot be adequately explained within the SDW-RPA scheme. The standard RPA result yields for $T > T_{\text{Néel}}$:

$$\chi_{\text{RPA}}^{+-}(\boldsymbol{k}, \omega) = \frac{\chi_0^{+-}(\boldsymbol{k}, \omega)}{1 - U\chi_0^{+-}(\boldsymbol{k}, \omega)}. \tag{5}$$

We note that the non-interacting susceptibility $\chi_0(\boldsymbol{Q}, 0)$ calculated for a two-dimensional finite system at half-filling exhibits a $1/T$ divergence as $T \to 0$. Therefore, there will always be a pole of the susceptibility at some non-zero temperature $T_{\text{Néel}}^{\text{RPA}}$, indicated by $U\chi_0(\boldsymbol{Q}, 0) = 1$, with a subsequent divergence of the total free energy of a finite system. This unphysical result is one of the consequences of an inherent shortcoming of the SDW-RPA treatment, namely, its failure to represent in a self-consistent manner the contribution

of the spin fluctuations to the free energy. The free energy can be expressed as a functional in the dynamical susceptibility [11] (see equations (8), (9)). On substituting expression (5) into this functional and subsequently differentiating it twice with respect to the staggered magnetization, one fails to recover the static limit of (5). This inconsistency has been pointed out [11] as the reason for predicting too high values for the Néel temperature of weakly antiferromagnetic metals. These arguments suggest the need to explore an analytic approach which would more adequately describe the thermodynamics of the system, if we are to try to relate our QMC results to any analytical concepts.

Such an approach has been developed as the theory of SCR by Moriya [11]. A renormalization function $\lambda$ is introduced which relates the exact sum of two-particle irreducible diagrams $\tilde{\chi}^{+-}_{UM}(\boldsymbol{k},\omega)$ to the free susceptibility $\chi^{+-}_{0M}(\boldsymbol{k},\omega)$ in a given background staggered magnetization $M$:

$$\tilde{\chi}^{+-}_{UM}(\boldsymbol{k},\omega)=\frac{\chi^{+-}_{0M}(\boldsymbol{k},\omega)}{1+\lambda_{UM}(\boldsymbol{k},\omega)}. \tag{6}$$

This renormalization function enters the calculation of the full susceptibility:

$$\chi^{+-}_{UM}(\boldsymbol{k},\omega)=\frac{\chi^{+-}_{0M}(\boldsymbol{k},\omega)\Lambda(\boldsymbol{k}+\boldsymbol{Q})+U[\chi^{+-}_{0M}(\boldsymbol{k},\boldsymbol{k}+\boldsymbol{Q},\omega)]^2}{\Lambda(\boldsymbol{k})\Lambda(\boldsymbol{k}+\boldsymbol{Q})-[U\chi^{+-}_{0M}(\boldsymbol{k},\boldsymbol{k}+\boldsymbol{Q},\omega)]^2} \tag{7}$$
$$\Lambda(\boldsymbol{k})\equiv 1+\lambda_{UM}(\boldsymbol{k},\omega)-U\chi^{+-}_{0M}(\boldsymbol{k},\omega).$$

Here the free Umklapp susceptibility at staggered magnetization $M$ is denoted by $\chi^{+-}_{0M}(\boldsymbol{k},\boldsymbol{k}+\boldsymbol{Q},\omega)$. The free energy of the system with $N_{\mathrm{el}}$ electrons is given by

$$F(U,M)=F_0(M)+\frac{U}{N}\left(\frac{N_{\mathrm{el}}^2}{4}-M^2\right)+\Delta F(U,M) \tag{8}$$

where the first two terms represent mean-field free energy and the third one is the correction due to the collective excitations which can be expressed via $\chi^{+-}_{UM}(\boldsymbol{k},\omega)$ as

$$\Delta F(U,M)=-T\int_0^U \mathrm{d}U'\sum_{\boldsymbol{k}\,\omega_\nu}\left[\chi^{+-}_{U'M}(\boldsymbol{k},\mathrm{i}\omega_\nu)-\chi^{+-}_{0M}(\boldsymbol{k},\mathrm{i}\omega_\nu)\right] \tag{9}$$

where $\omega_\nu=2\pi T\nu$. The sum in (9) is dominated by $\chi^{+-}_{UM}(\boldsymbol{Q},0)$, which justifies making the long-wavelength static approximation $\lambda_{UM}(\boldsymbol{k},\omega)=\lambda_{UM}(\boldsymbol{Q},0)$. In this approximation, equations (7)–(9) together with the thermodynamical relation between the static susceptibility and the free energy:

$$\frac{1}{\chi^{+-}_{UM}(\boldsymbol{Q},0)}=\frac{1}{2}\frac{\partial^2 F(U,M)}{\partial M^2}\Big|_{M=0} \tag{10}$$

constitute a set of equations for the susceptibility, automatically maintaining the self-consistency requirement. Equation (10) can be solved by expanding $\lambda_{UM}(\boldsymbol{Q},0)$ in powers of $M$. In the next-to-leading-order expansion: $\lambda_{UM}(\boldsymbol{Q},0)\approx\lambda_0(U)+(1/2)\lambda_2(U)M^2$, we obtain

$$\lambda_0(U)=\chi^{+-}_{0M}(\boldsymbol{Q},0)\frac{\partial^2\Delta F}{\partial M^2}\Big|_{M=0}$$
$$\lambda_2(U)=\frac{\partial^2\chi^{+-}_{0M}(\boldsymbol{Q},0)}{\partial M^2}\frac{\partial^2\Delta F}{\partial M^2}\Big|_{M=0}. \tag{11}$$

Since even within this approximation the thermodynamics of the spin fluctuations is accounted for self-consistently, the qualitative description of the susceptibility is likely to be more accurate than the one provided by the SDW-RPA treatment. Apparently, due

to the finite-size $1/T$ divergence of $\chi_0$, Moriya's approximation of $\lambda$ being independent of $U$ and $M$, used in the infinite-system calculation [11], is too crude for this calculation. By substituting the solution of equation (11) for $\lambda_{UM}(\boldsymbol{Q}, 0)$ into (6) at $\omega = 0$, we obtain the value of $\tilde{\chi}^{+-}_{U0}(\boldsymbol{k}, 0)$. The static susceptibility (for $T > T_{\text{Néel}}$) is obtained by replacing $\chi^{+-}_0(\boldsymbol{k}, 0)$ in equation (5) by $\tilde{\chi}^{+-}_{U0}(\boldsymbol{k}, 0)$ (figure 2). The calculation of the direct and Umklapp free susceptibility entering equation (7) was done for lattice sizes $8^2$ and $10^2$. Thus the finite-size effects, inevitably present in the QMC simulations, have been taken into account in the analytical calculation. Unlike RPA-SDW treatment results, SCR results are in principle comparable with the finite-cluster QMC simulations. While exhibiting strong enhancement of the static susceptibility at the nesting vector, the SCR value remains finite, in agreement with the QMC result, and as expected for a finite system. Due to the discrete spectrum of single-particle excitations on a finite lattice, $\chi''_0(\boldsymbol{k}, \omega)$ is a sequence of $\delta$-functions, and becomes smooth only for an infinite system. An imaginary regularizer (corresponding to a finite lifetime for a quasiparticle) has thus to be introduced to allow the calculation of the dynamical susceptibility using equation (7). We found the results to be sensitive to the value of this regularizer, therefore, a meaningful comparison with the QMC data can be made only for static susceptibility. The extension of Moriya's theory presented here leads to qualitative agreement with the QMC values. The quantitative difference of approximately a factor of 2 (see figure 2) seems to be a consequence of the pole structure of the expression for the susceptibility, obtained upon substituting equation (6) into equation (5). Thus the approximations made in the evaluation of the renormalization function $\lambda$ may account for this quantitative discrepancy. This shortcoming noted, we emphasize that our calculations were done with no parameter adjustment.

Making a standard approximation, $\chi'(\boldsymbol{q} + \boldsymbol{Q}, 0) = \chi'(\boldsymbol{Q}, 0)/(1 + \xi^2\boldsymbol{q}^2)$, for small deviations $\boldsymbol{q}$ from the nesting vector, we obtain the correlation lengths $\xi = 3.0a$ and $\xi = 3.4a$ ($a$ being the lattice spacing) for the $8^2$ and $10^2$ lattices respectively. The SCR estimates $\xi = 3.9a$ and $\xi = 4.4a$ are similar in their values and in the finite-size effects exhibited. We emphasize, however, that since the correlation length calculated is of the order of the lattice linear dimension, this estimate can vary as the lattice size increases.

To summarize, the SVD technique is applicable to the derivation of the dynamical properties of collective excitations in SCES. The dynamical susceptibility obtained from QMC simulations contradicts the qualitative predictions of the SDW-RPA treatment; in particular there is no evidence for SDW gap formation in the longitudinal time-ordered correlation function. Therefore it is unlikely that the gaps observed for this lattice size and temperature in previous QMC simulations of the single-particle density of states [7] can be explained within the SDW-RPA, as was indeed pointed out in reference [8]. We note that on comparing the SVD analytic continuation for the spin dynamics with a maximum-entropy calculation, we found no qualitative discrepancy between them, in contrast to the result of a similar comparison for the case of single-particle spectral weight. Our results support the evidence for the insufficiency of the SDW-RPA picture for describing the spectrum of excitations of the Hubbard model [16, 17]. Attempts to fit QMC results to SDW-RPA predictions can be misleading. The qualitative agreement in the static limit with the SCR calculation points to the importance of including the paramagnon interaction in the description of the magnetic properties of the Hubbard model. This approach has previously been used to obtain, on a more phenomenological basis, the dynamics of collective excitations in HTSC compounds in the normal phase, as well as to calculate the pairing potential [3]. Our work outlines a way of examining these properties directly from the lattice-field model by means of numerical simulations as well as by a power series expansion in the magnetization within the SCR theory.

We are grateful to J H Jefferson, G Aeppli, A Bratkovsky and V Kabanov for stimulating discussions. This research was funded by an SERC grant GR/J18675, and our general development of SVD techniques by the US Army Research Office, agreement No DAAH04-995-1-0280. Two of the authors (CEC and PEK) were supported by the EPSRC and ORS–University of London respectively.

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