

## Single-hole spectral function and spin-charge separation in the $t$ - $J$ model

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Worm algorithm Monte Carlo simulations of the hole Green function with subsequent spectral analysis were performed for  $0.1 \leq J/t \leq 0.4$  on lattices with up to  $L \times L = 32 \times 32$  sites at a temperature as low as  $T = J/40$ , and present, apparently, the hole spectral function in the thermodynamic limit. Spectral analysis reveals a  $\delta$ -function-sharp quasiparticle peak at the lower edge of the spectrum that is incompatible with the power-law singularity and thus rules out the possibility of spin-charge separation in this parameter range. Spectral continuum features two peaks separated by a gap  $\sim 4 \div 5 t$ .

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For almost four decades the problem of hole dynamics in magnetic systems has attracted constant interest with applications ranging from properties of charge carriers in magnetic semiconductors and insulators<sup>1,2</sup> to vacancies in solid <sup>3</sup>He.<sup>3</sup> The research in this area exploded with the discovery of high-temperature superconductors in cuprates, where superconductivity appears upon light doping of antiferromagnetic (AFM) insulators. Despite an enormous theoretical effort over the years and quite a variety of treatments (for reviews, see, e.g., Ref. 4) a complete solution of this inherently strong-coupling problem still does not exist, especially in the most interesting region of  $t > J$ , where  $J$  is the exchange coupling constant and  $t$  is the hopping matrix element in the  $t$ - $J$  Hamiltonian

$$H = -t \sum_{\langle ij \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + J \sum_{\langle ij \rangle} \left( \mathbf{s}_i \cdot \mathbf{s}_j - \frac{1}{4} n_i n_j \right). \quad (1)$$

Here,  $c_{j\sigma}$  is projected (to avoid double occupancy) fermion annihilation operator,  $n_i = \sum_\sigma c_{i\sigma}^\dagger c_{i\sigma} \neq 2$  is the occupation number,  $\mathbf{s}_i = \sum_{ss'} c_{is}^\dagger \boldsymbol{\sigma}_{ss'} c_{is'}$  is spin-1/2 operator, and  $\langle ij \rangle$  denote nearest-neighbor sites of the two-dimensional (2D) square lattice.

The central problem in the hole dynamics is whether or not its spin and charge degrees of freedom separate. The standard way to answer this question is to study the spectral function  $A_{\mathbf{p}}(\omega) = -\pi^{-1} \text{Im} G_{\mathbf{p}}(\omega)$ , where  $G_{\mathbf{p}}(\omega)$  is the hole Green function. If there is an elementary excitation associated with the hole, the spectral function is supposed to feature a peak at the lower edge of the spectrum. What is crucial, however, is not the presence of the peak itself, but its functional form.<sup>5,6</sup> Within the self-consistent Born approximation scheme (SCBA) (Ref. 7) one finds finite overlap between the bare hole and low-energy quasiparticle states, which means that the peak is  $\delta$  functional and the hole is described as coherently propagating spin polaron in the nearly ordered antiferromagnetic (AFM) background (with vanishing scattering at low temperature due to small density of spin waves).<sup>7</sup>

In contrast to that, various resonating-valence-bond descriptions and Anderson's general arguments about the breakdown of the Fermi-liquid picture in the system with

nodouble-occupancy constraint (see, e.g., Ref. 8) strongly suggest that power-law singularity, which is indicative of a spin-charge separation scenario, might be the case (there is even a claim that the quasiparticle weight  $Z$  should be rigorously zero)<sup>9</sup>. To make the issue more confusing, angle-resolved photoemission spectroscopy experiments<sup>10,11</sup> show very broad maximum in  $A(\omega)$ , which can be considered both as the quasiparticle peak with anomalously large broadening or as the evidence for the composite nature of quasiparticles.<sup>12</sup>

The quasiparticle picture was supported by exact calculations on small clusters,<sup>4,13,14</sup> but system sizes (up to 32 sites) were too small to perform finite-size scaling. Variational calculations, Green-function Monte Carlo and density-matrix renormalization-group studies were mostly concerned with the dispersion law  $\epsilon_{\mathbf{k}}$  (lowest energy in a given momentum sector). Large scale simulations of the imaginary time Green function  $G_{\mathbf{k}}(\tau)$  were performed recently using a combination of the loop-cluster Monte Carlo method for the AFM state and hole evolution in the fixed space-time spin background.<sup>15</sup> This method works only for relatively large exchange  $J > 0.6 t$ , since a magnetic background is simulated *without* the hole and polaron-type distortions have to be accounted for as quantum fluctuations *before* the hole is introduced. For  $J/t < 0.6$ , the error bars in  $G_{\mathbf{k}}(\tau)$  are too large for a reliable spectral analysis (see below).

To summarize, we still lack evidence that for small  $J$ , the quasiparticle weight remains finite in the thermodynamic limit and the lowest peak has nothing to do with the power-law singularity. We thus find it important to rule out the possibility that the  $t$ - $J$  model may explain the data of Refs. 10, 11 (as suggested by Ref. 9), so that extensions of the model such as  $t'$  and  $t''$  terms<sup>16</sup> or frustrating exchange couplings are proven necessary.

Speaking classically, moving hole breaks AFM bonds, and thus, its energy increases linearly with the travel distance<sup>2,17</sup> (this consideration, or the string-potential picture, is most appropriate for the  $t$ - $J_z$  model). It is believed that the ground energy scaling  $E_{\mathbf{k}_0} \sim J^{2/3}$  [where  $\mathbf{k}_0 = (\pi/2, \pi/2)$ ] and excitation spectrum are described by the string-potential picture,<sup>4,7,13,15,18,19</sup> and transverse spin fluctuations do not "erase" strings completely. In the limit of

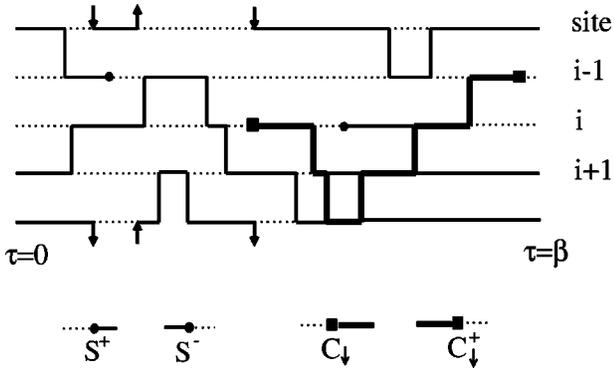


FIG. 1. World-line configuration describing quantum AFM with the hole; solid (dotted) lines correspond to spin-up (-down) states and the bold line describes the hole. Arrows indicate how periodic boundary conditions are used.

small  $J$ , the theory predicts that several resonances in  $A(\omega)$  have to be seen with the peak positions being strictly related to the eigenvalue properties of Airy functions. Early exact diagonalization studies on clusters  $4 \times 4$  (Ref. 4) attributed two peaks above the ground state to string resonances, however later studies on larger clusters<sup>13,14</sup> were not able to detect the second resonance, and the spectral function was showing strong size dependence. What happens at small  $J$  in the thermodynamic limit remains an open question.

In this report, we present results for  $G_{\mathbf{k}}(\tau)$  and  $A_{\mathbf{k}}(\omega)$  obtained from Monte Carlo simulations on systems with  $16 \times 16$  and  $32 \times 32$  sites and at temperatures as low as  $T/J = 0.025$  (for the largest system size) using continuous-time Worm algorithm<sup>20</sup> in combination with the recently developed spectral analysis, which is capable of resolving infinitely sharp features in  $A(\omega)$ .<sup>21</sup> The method itself is free from any systematic errors, and we were unable to detect finite-size corrections in our data; thus, we believe, our results describe correctly the thermodynamic limit. In the parameter range studied  $0.1 \leq J/t \leq 0.4$ , the lowest peak in  $A_{\mathbf{k}_0}(\omega)$  is a  $\delta$  function within the resolution limit of order of  $0.01 \div 0.03 t$ , which means that our quasiparticle is the spin-polaron. For the excitation spectrum we observe two well-separated peaks for all values of  $J$ . The ground state energy scaling does follow the  $J^{2/3}$  law predicted by the string-potential theory. Although we were unable to resolve individual string resonances, we believe that their combined effect is seen as the first peak in the spectral continuum since its position also scales as  $J^{2/3}$ . The high-energy peak is roughly at a constant distance  $\sim 5t$  from the ground state.

Worm algorithm is based on the idea that world-line configurations of spins and the hole are updated through the space-time motion of the creation and annihilation operators. In Figs. 1 and 2 we show the typical configuration of the Heisenberg AFM with the hole, and Monte Carlo updates that apply to it. Physical configurations contributing to the hole Green function are those that have no spin end points (denoted by filled circles).

Since the world-line representation is based on the expansion of the statistical evolution operator  $e^{-H/T}$  in powers of  $t$  and  $J$ , it suffers from the sign problem that first appears in

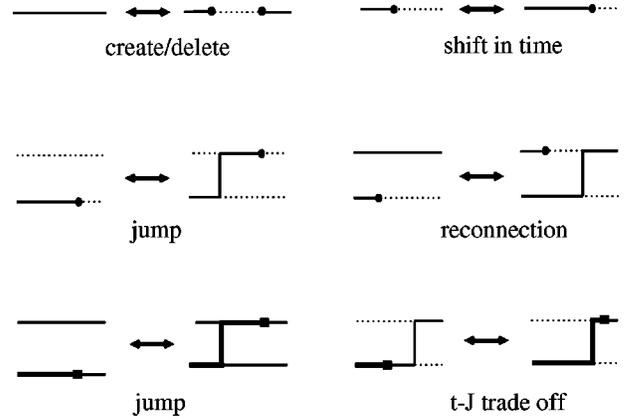


FIG. 2. Elementary Monte Carlo updates that form an ergodic set. We show updates for  $s^+$  and  $c_{\uparrow}^{\dagger}$  end points only since procedures for  $s^-$  and  $c_s^{\dagger}$ ,  $c_s$  are identical up to a change of notations (i.e., using proper incoming and outgoing lines).

order  $t^2 J^3$  (see Fig. 3). It is worth noting that if not for the sign problem, spin-charge separation can be ruled out by the analysis of world-line configurations. Let the hole be created by the  $c_{i\downarrow}$  operator. If spin-charge separation does take place, one should see, following the evolution of the system configuration in imaginary time, an extra spin density leaving the hole creation site and going into the bulk, i.e., the world-line density far from the hole should increase. At  $T=0$ , the AFM ground state is ordered (as opposite to the spin liquid state) and the minimal possible change in the world-line density is equivalent to having exactly one extra world line, which can be traced out and interpreted as spin-one magnon excitation. We may now construct an operator that has finite overlap with the quasiparticle excitation as a product  $s^- c_{\downarrow}$ , where  $s^-$  is added to cancel the extra magnon in the bulk. However, up to a single hopping transition the above composite operator is identical to  $c_{\uparrow}$ , and we conclude that holes are good quasiparticles in contradiction with the original assumption (probably rephrasing the proof of Ref. 7).

However, in the presence of the sign problem, the above consideration should be taken with extreme caution. It may turn out that ordered world-line configurations compensate each other completely and single-configuration conclusions are misleading, as suggested in Ref. 9 where the hole-related sign problem is called the ‘‘irreparable phase string effect’’ and argued to cause spin-charge separation.

The sign problem implies that we may not calculate  $G(\tau)$  reliably over long time scales and have to restrict our simulation to  $t\tau < 3 \div 4$  to suppress sign fluctuations by larger statistics. Fortunately, on this time scale  $G_{\mathbf{k}}(\tau)$  is already in its asymptotic regime and the data are sufficiently accurate to

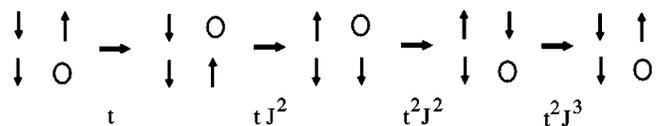


FIG. 3. The lowest order (in  $t$  and  $J$ ) transformation leading to the sign problem.

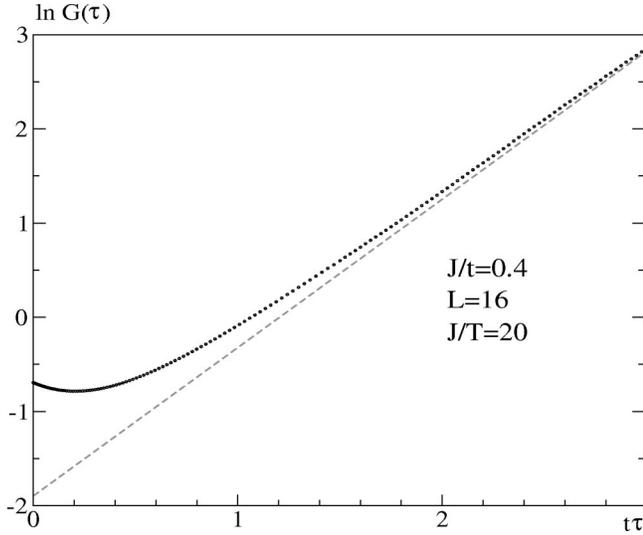


FIG. 4.  $G_{\mathbf{k}_0}(\tau)$  (circles) and the asymptotic line  $Z_{\mathbf{k}_0} e^{-E_{\mathbf{k}_0} \tau}$  (dashed) for  $J/t=0.4$  with  $Z_{\mathbf{k}_0}$  and  $E_{\mathbf{k}_0}$  obtained from the weight and position of the peak in the spectral function.

reveal the ground-state properties. Formally, calculations are done at finite  $T$  but its value is more than an order of magnitude smaller than the energy of the lowest magnon state in a given system size. For each value of  $J$ , the calculation time was about two weeks on a PIII-600 workstation.

In Fig. 4 we show simulated  $G_{\mathbf{k}_0}(\tau)$  for  $J/t=0.4$  and the asymptotic law  $Z_{\mathbf{k}_0} e^{-E_{\mathbf{k}_0} \tau}$  with the quasiparticle weight and ground-state energy obtained from the weight and position of the  $\delta$  peak in  $A_{\mathbf{k}_0}(\omega)$ . Note that for small values of  $J$ , the data have to be very accurate to describe correctly how  $G(\tau)$  approaches its asymptotic behavior  $G_{\mathbf{k}_0} \rightarrow Z_{\mathbf{k}_0} e^{-E_{\mathbf{k}_0} \tau}$ . Error bars are shown but are smaller than the symbol size (the relative accuracy is better than  $10^{-2}$  even for points with the largest  $\tau$  where the sign problem was the most severe).

The spectral analysis of  $G_{\mathbf{k}_0}(\tau)$  was done using stochastic optimization procedure developed earlier for the polaron problem.  $A(\omega) = N^{-1} \sum_{i=1}^N A_i(\omega)$  is obtained as an average over spectral densities that optimize deviations between  $G(\tau)$  and  $\int d\omega e^{-\omega \tau} A_i(\omega)$ . The parameter space of  $A_i(\omega)$  is defined by the step-wise constant functions, which, in particular, includes infinitely sharp peaks and is not associated with any predefined set of frequencies<sup>21</sup> (it is known that  $\delta$  peaks cannot be handled satisfactorily by the maximum entropy method<sup>15,22</sup>).

In Fig. 5 we show our results for  $A_{\mathbf{k}_0}(\omega)$  calculated at points  $J/t=0.4, 0.2, 0.1$ . We clearly see a  $\delta$ -sharp peak at the lower edge of the spectrum. The structure of this peak is incompatible with the power-law singularity since its width is smaller than the lowest-magnon excitation in our system [for  $J/t=0.4$ , the quasiparticle peak width is only  $0.01 t$  (!) while the natural scale for the power law is set by  $J$ ]. This is the central result of our paper which conclusively rules out spin-charge separation scenario for the single hole dynamics in the  $t$ - $J$  model and confirms finite quasiparticle weight in the thermodynamic limit. To verify that finite-size and finite-

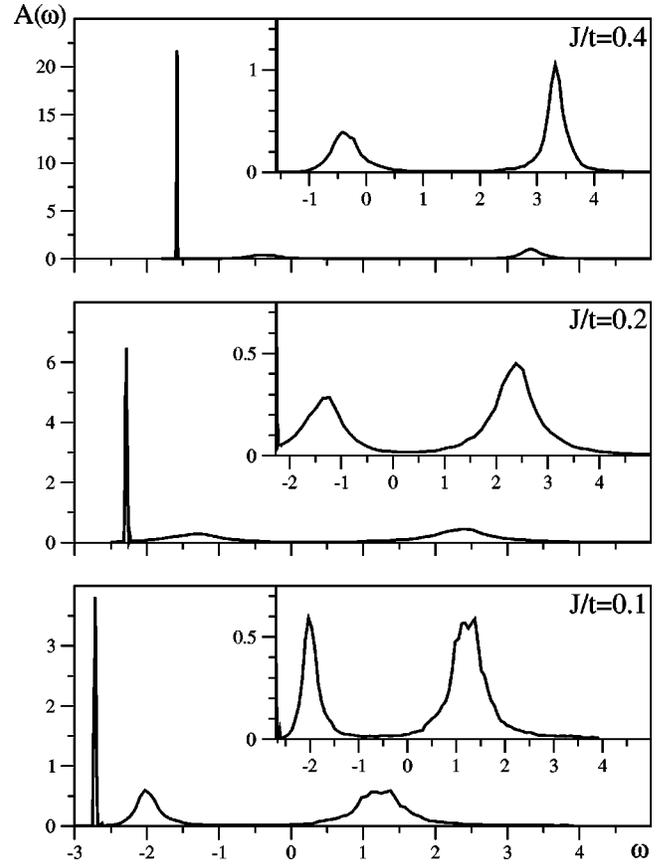


FIG. 5. Spectral functions for  $J/t=0.4, 0.2,$  and  $0.1$ . Frequency is measured in units of  $t$  and the integral  $\int d\omega A(\omega)$  is normalized to unity. These spectra were obtained for the  $16 \times 16$  lattice at  $T = J/20$ .

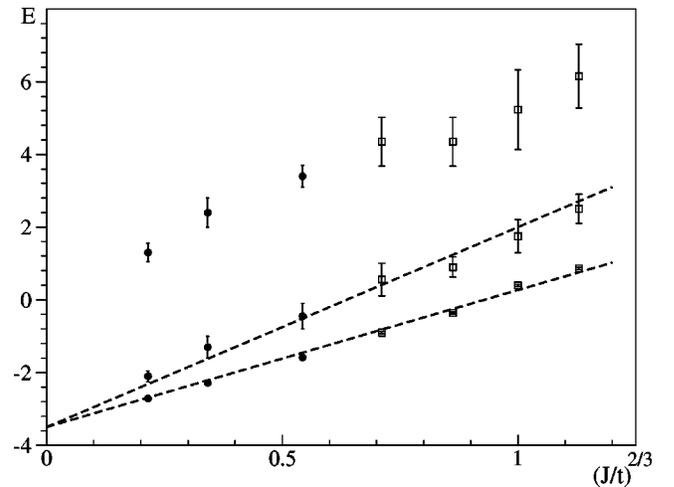


FIG. 6. Peak positions as functions of  $(J/t)^{2/3}$ . Data points for  $J > 0.4$  (squares) were taken from Ref. 15 [for  $J=0.4$   $t$ , the second peak was not resolved in Ref. 15 because of large error bars in  $G(\tau)$ ]. The two lines are fits  $y(x) = a + b(J/t)^{2/3}$  with  $a = -3.5 t$ ,  $b = 3.77 t$  for the ground state, and  $b = 5.5 t$  for the first peak in continuum.

temperature corrections are negligible, we performed long-time simulations in a  $32 \times 32$  lattice at temperature  $T=J/40$  for  $J/t=0.2$ , but within the error bars,  $G(\tau)$  was indistinguishable from the result obtained for  $L=16$  and  $T=J/20$ . Our final result for the quasiparticle weight is  $Z(J=0.4)=0.150(7)$ ,  $Z(J=0.2)=0.10(1)$ ,  $Z(J=0.1)=0.05(1)$ , which agrees with SCBA calculations<sup>7</sup> in this parameter range.

Unfortunately, the ill-defined problem of numeric analytic continuation does not allow us to study fine structures in the spectral density, especially if they are “screened” by low- and high-frequency peaks. [The low-frequency peak is fixed by the long-time behavior of  $G(\tau)$ , while the high-frequency peak is fixed by the short-time decay of  $G(\tau)$  where the data are extremely accurate.] Our tests show that multiple peaks in the middle cannot be resolved by spectral analysis even when we use analytically exact  $G(\tau)$  data. It means that the

absence of multiple string resonances above the ground state in our results for  $A(\omega)$  may not be considered as a proof that string potential picture fails in the quantum case. We would rather consider the second peak as a “course grain” description of spectral density at intermediate energies. However, if string excitations do exist, their combined effect should be seen as the  $J^{2/3}$  scaling law for the peak position. In Fig. 6 we plot peak positions as functions of  $(J/t)^{2/3}$  for  $0.1 \leq J/t \leq 1.2$  with error bars obtained as peak half-widths. We conclude that for the second peak, the scaling law is obeyed within the error bars. The high-energy peak stays roughly at a constant distance from the ground state, and clearly, the physics behind it is different.

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