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Spectral function of the two-dimensional Hubbard model: A density matrix renormalization group plus cluster perturbation theory study

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We study the spectral function of the two-dimensional Hubbard model using cluster perturbation theory, and a density matrix renormalization group as a cluster solver. We reconstruct the two-dimensional dispersion at and away from half-filling using $2 \times L$ ladders, with L up to 80 sites, yielding results with unprecedented resolution in excellent agreement with quantum Monte Carlo. The main features of the spectrum can be described with a mean-field dispersion, with kinks and pseudogap traced back to scattering between spin and charge degrees of freedom.

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I. INTRODUCTION

Mott insulators defy conventional paradigms, since the rigid band picture behind the physics of semiconductors does not apply: in strongly interacting systems, the bands change with doping, giving rise to a complex phenomenology that includes hole pockets, Fermi arcs, and kinks [1–4]. The spectral properties near the Mott transition in the Hubbard model have been studied extensively by a number of computational techniques [5–37] and results indicate the emergence of excitations in the Mott gap at finite doping. The "leaking" of spectral weight into the gap has been explained a while ago by a seminal work by Eskes *et al.* [38], reviewed in Ref. [39].

Previous numerical studies using cluster perturbation theory (CPT) [35] indicate the survival of one-dimensional aspects in the spectrum of the fully two-dimensional system, and suggest that some of the features observed in the experiments, such as kink or waterfalls [1], could be attributed to spin-charge separation and traced back adiabatically to spinon and holon dispersion in one-dimensional chains.

In one-dimensional (1D) systems, the Fermi-liquid picture breaks down: the natural excitations are described by Luttinger liquid theory [40–42] as collective bosonic modes carrying spin and charge, with each degree of freedom being characterized by a different energy scale. Even though spin-charge separation is intrinsically a manifestation of 1D physics, the possibility of its presence in two dimensions or quasi-two-dimensional (quasi-2D) systems has been extensively debated, particularly within the context of high-temperature superconductivity [43]. Some numerical studies in this direction, looking at two, three, and four-leg t-J ladders, indicate the presence of spinon and holon excitations [44–48]. Whether spin-charge separation, or electron-phonon interactions are responsible for the unexpected spectral features such as kinks, and "waterfalls" in cuprates, is still open to interpretation and a topic of great debate.

Since CPT relies on the solution of small clusters, it cannot describe long-range order. These shortcomings can be overcome by using an extension of the method called the variational cluster approximation (VCA) also referred to as VCPT. The VCA extends the previous ideas by incorporating additional ingredients, such as external fields, or even additional cluster sites, and introducing a variational principle to self-consistently determine the optimal symmetry-breaking fields [22,25,49–52]. The variational principle is derived from a general framework, the self-energy functional approach, that has the power to unify several cluster methods, including cluster (or cellular) dynamical mean field theory [53] and the dynamical cluster approximation (DCA) [54,55], under the same mathematical structure [56].

In this work, we use the time-dependent density matrix renormalization group method (tDMRG) [57–60] as a solver for CPT, and study the spectral function of the 2D Hubbard model with unprecedented resolution at and away from half-filling. The tDMRG allows us to couple clusters that are already infinite (very large) in one spatial dimension, representing a tremendous advance over traditional calculations with small clusters, with typically 12–16 sites.

In Sec. II we introduce the methods, in Sec. III we describe and analyze the results, and we conclude with a discussion.

II. METHODS

CPT is a technique that applies to problems with local interactions, such as the Hubbard model [18,20,61]. It provides an approximation to the single-particle Green's function of the problem in the thermodynamic limit by coupling clusters of small size in a variant of strong coupling perturbation theory. The main idea consists in dividing the lattice into small clusters which can be solved exactly, and coupling them together to reconstruct the original system. The single-particle Green's function for the thermodynamic limit is constructed by solving a simple Dyson-like equation:

$$\mathbf{G}^{-1} = \mathbf{G}'^{-1} - \mathbf{T}, \tag{1}$$

where the bold symbols represent matrices: $\mathbf{G}$ is the Green's function we seek, $\mathbf{G}'$ is the Green's function in the cluster, and $\mathbf{T}$ is a hopping matrix connecting the clusters. In the following we assume that the symbol G refers to *retarded* Green's functions.

In this work, our cluster consists of a $2 \times L$ ladder, and the model is given by the usual Hubbard Hamiltonian:

$$H = -t \sum_{i,\lambda,\sigma} (c^\dagger_{i,\lambda\sigma} c_{i+1,\lambda\sigma} + \text{H.c.}) - t \sum_{i,\sigma} (c^\dagger_{i2\sigma} c_{i1\sigma} + \text{H.c.}) + U \sum_{i,\lambda} n_{i,\lambda\uparrow} n_{i,\lambda\downarrow}, \tag{2}$$

where the operator $c^{\dagger}_{i\lambda\sigma}$ creates an electron on rung i and leg $\lambda = 1,2$ with spin σ,$n_{i\lambda\sigma}$ is the electron number operator, and t and U parametrize the hopping and Coulomb repulsion, respectively. In the following we assume periodic boundary conditions in the leg direction, and we will address the finite size effects in the technical discussion below.

Since the cluster possesses translational invariance along the leg direction x, we can readily Fourier transform our Green's functions as:

$$G'_{\lambda\lambda'}(k_x) = \sum_n e^{ik_x na} G'_{\lambda\lambda'}(x),$$

where a is the lattice spacing, $x = na$, and we have omitted the spin index, since our problem is also invariant under a spin inversion. This expression defines a Green's function in a hybrid representation, since the leg index λ still represents a real space coordinate. However, Eq. (1) is diagonal in k_x, meaning that G is a 2×2 matrix for each value of k_x, which is exactly equivalent to solving the CPT equations for a two-site cluster:

$$G^{-1}_{\lambda,\lambda'}(k_x,Q,\omega) = G'^{-1}_{\lambda,\lambda'}(k_x,\omega) - T_{\lambda,\lambda'}(Q),$$

with

$$T_{\lambda,\lambda'}(Q) = -t[e^{iQ}\delta_{\lambda,2}\delta_{\lambda',1} + e^{-iQ}\delta_{\lambda,1}\delta_{\lambda',2}]$$

and $Q = 2k_y$ introducing the dependence on k_y. By restoring the quasitranslational invariance, we obtain the CPT Green's function as

$$G^{CPT}(k_x,k_y,\omega) = \frac{1}{2}\sum_{\lambda,\lambda'=1}^{2} e^{-ik_y(\lambda-\lambda')} G_{\lambda,\lambda'}(k_x,2k_y,\omega). \quad (3)$$

In addition, by symmetry we obtain $G_{11} = G_{22}$ and $G_{21} = G_{12}$, which reduces the number of required simulations. These equations are clearly very simple, and the main challenge consists in calculating the Green's functions with tDMRG, which can be readily done using well established methods, extensively described in the literature [59], and reviewed in Ref. [60]. The tDMRG method yields the single-particle correlation function in real space and time, and the Green's functions are obtained by Fourier transforming the results to momentum and frequency. The most subtle aspect of the calculation concerns the use of open boundary conditions along the x direction. As discussed in Refs. [57,59,62], the finite size effects introduced by the boundaries can be controlled in two ways: by convolving the Fourier transform to momentum space with a smooth window that vanishes at the boundaries, and by limiting the simulation time to prevent reflections at the two ends of the ladder. In addition, to avoid artifacts such as "ringing" in the Fourier transform to frequency, we also convolve the results with a Hann window along the time direction. This has the effect of introducing an artificial broadening in the spectral function that is inversely proportional to the width of the time window. Long simulation time would reduce the broadening in frequency, with the price of introducing ringing. These features are amplified when the matrix is inverted and plugged into the CPT equation, introducing instabilities that result, for instance, in negative values of the spectral function. Therefore, our simulation time (and Hann window width) is relatively short, $t_{\max} \sim 15$ in units of the inverse hopping, and makes the use of linear prediction methods to extrapolate in time [63] completely unnecessary.

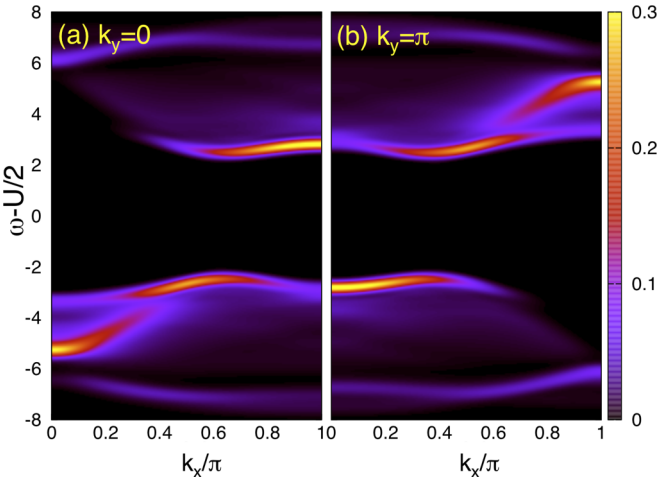

FIG. 1. Spectral function of a Hubbard ladder with $L = 80$ and $U/t = 8$, at half-filling, obtained with tDMRG. Panels (a) and (b) show the symmetric and antisymmetric sectors, respectively, which are related by particle-hole symmetry.

III. RESULTS

We have simulated a 2×80 Hubbard ladder with 600 DMRG states, and using a time window of width $\Delta t = 15$, a time step $\delta t = 0.02$, and a third order Suzuki-Trotter decomposition of the evolution operator. (In the following, we take $t = 1$ as our unit of energy.) In Figs. 1(a) and 1(b) we show results for the bare spectral function of the ladder (before CPT), at half-filling and for $U/t = 8$, as a function of k_x, and for the symmetric and antisymmetric sectors, represented by $k_y = 0,\pi$, respectively:

$$G'(k_x,k_y = 0,\pi,\omega) = G'_{11}(k_x,\omega) \pm G'_{12}(k_x,\omega),$$

where the $\pm$ signs correspond to the two values of k_y. Interestingly, the truncation errors are very small, of the order of 10^{-7}, which can be explained by noticing that the cluster is gapped in both the charge and spin sectors. Curiously, and to the best of our knowledge, there are no results with DMRG for this ladder system in the literature, probably stemming from previous observations that *dynamical* DMRG [64–66] is computationally very expensive in this geometry, and only recently has it been applied to t-J ladders [67].

Even though ladders are quasi-one-dimensional systems with spin-charge separation and Luther-Emery behavior [68,69], the sharp features observed in chains, such as shadow and spinon bands, are washed out and less discernible, with most of the spectral weight concentrated in the holon bands. The spinon band in the lower Hubbard band (LHB) for $k_y = 0$ shows a tendency to merge with the holon band and forms a single quasiparticle dispersion, as one would expect from a Fermi liquid. The dispersion presents a waterfall that resembles a discontinuity in the dispersion at $k_x = \pi/2$, and could be attributed to a mixing between the charge and spinon modes. The upper Hubbard band (UHB) displays a sharp spinonlike dispersion centered at $k_x = \pi$ with very small

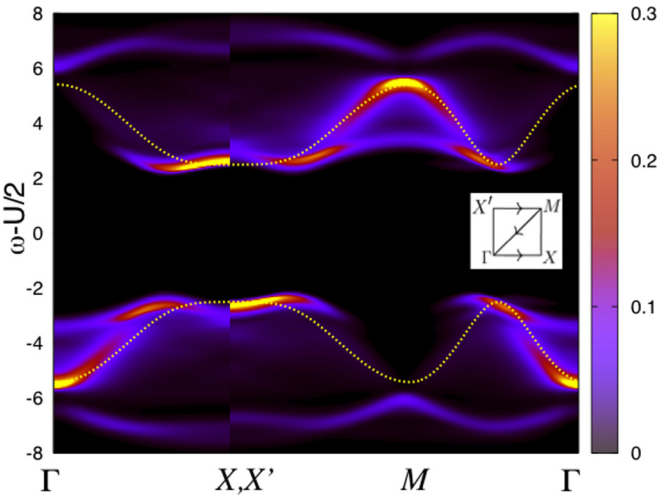

FIG. 2. CPT spectral function of the $U = 8$ 2D Hubbard model at half-filling obtained using a 2×80 ladder as a cluster, and tDMRG as a solver. The dashed line shows the Hartree-Fock dispersion.

bandwidth. These features are reversed for $k_y = \pi$: Due to particle-hole symmetry, the bands are reflected about the Fermi energy and shifted in k_x by π.

In Fig. 2(a), we present the tDMRG+CPT spectral function of the 2D Hubbard model at half-filling with $U/t = 8$ along the $\Gamma \rightarrow X \rightarrow M$ path in the Brillouin zone. The CPT equations along the $X \rightarrow M$ line will produce a mixture of $G'_{11}(\pi,\omega)$ and $G'_{12}(\pi,\omega)$. The small cluster size in the transverse direction yields very limited resolution along this line. However, in a rotational invariant lattice, they should be identical to the results for the $k_y = \pi$ boundary of the Brillouin zone, which can be obtained with very high resolution. For this reason, we have plotted the CPT spectrum for the $k_y = \pi$ along the $X \rightarrow M$ segment, with the price of introducing an artificial discontinuity at the X point.

The spectrum shows an uncanny resemblance to the ladder's, albeit with a weak renormalization. As explained in Ref. [35], the CPT introduces a shift of spectral weight at high energies while keeping the spectral weight near the Fermi level almost unaffected, which makes the holonlike bands sharper and the spinonlike bands weaker, yielding a dispersion that resembles that of quasiparticles. The spinon features remain as an incoherent background *at low energies*, while preserving the waterfall at $(\pi/2,\pi/2)$.

Following Ref. [16], the quasiparticle dispersion can be fitted by a mean-field (Hartree-Fock) dispersion assuming a Néel antiferromagnetic (AFM) order [16,70], given by the two bands

$$E_{\pm}(\mathbf{k}) = \pm\sqrt{[-2\tilde{t}(\cos k_x + \cos k_y)]^2 + \tilde{\Delta}^2},$$

as shown by the dashed line in the figure, where we take the gap $\tilde{\Delta}$ and $\tilde{t}$ as free fitting parameters. This indicates that, despite its low dimensionality, the ladder cluster already introduces features in the spectrum that contain information about the onset of AFM order. Moreover, the spectral function displays a remarkable agreement with the quantum Monte Carlo (QMC) results from Refs. [10,11,15,16] but with much better resolution. In particular, we observe similar features

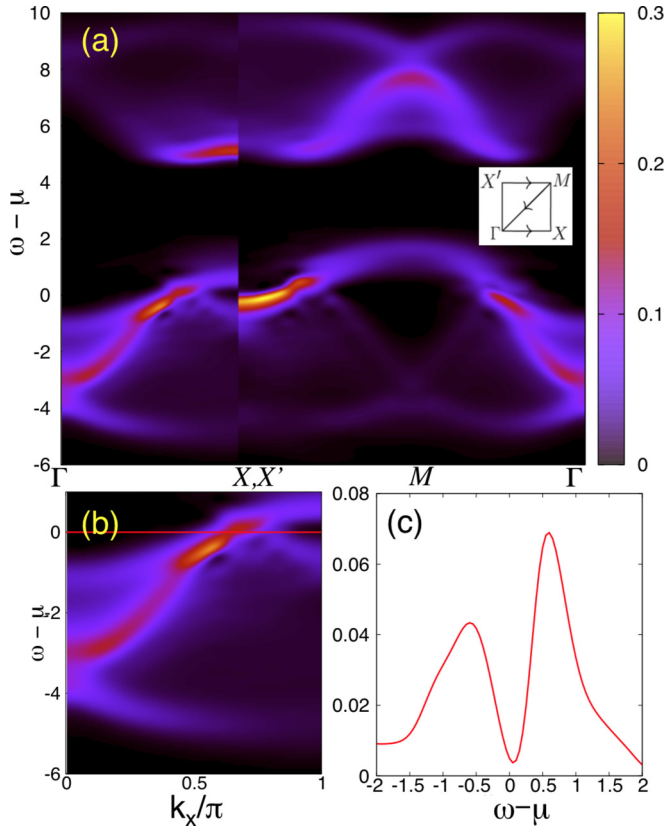

FIG. 3. (a) CPT spectral function of the doped $U = 8$ 2D Hubbard model obtained using a 2×40 ladder as a cluster, with $n = 72$ electrons. (b) Same results focusing on the kink and the pseudogap region along the $\Gamma \rightarrow X$ line. (c) Pseudogap at the X point.

such as the flat dispersion in the UHB and LHB centered at the $(\pi,0)$ point, and the weak spinonlike incoherent background at low energies. The high-energy "bands" observed in QMC can be associated to the shadow bands in the ladder dispersion, echoes of one-dimensional physics. Remarkably, these same features are also obtained using square clusters with CPT [35], and VCPT [22,25], after introducing an external staggered field to induce antiferromagnetic correlations in 2D clusters. Putting together the results from this and previous works, the evidence indicates that (i) these features are not artifacts of the quasi-one-dimensional ladder, and (ii) they survive in the presence of long-range order.

We now shift our attention toward the doped case. In Fig. 3(a) we show a similar calculation for a 2×40 ladder with 72 electrons, corresponding to 10% doping, which also keeps us away from any charge-density wave instabilities. We used a smaller cluster and more states ($m = 1000$), since now the charge sector is gapless and introduces more entanglement in the problem, making the simulations computationally more expensive.

The spectrum looks very similar to the CPT results in small clusters [35]: the waterfall is no longer a discontinuity but a continuous feature resembling a "kink," and there is clear transfer of spectral weight above the Fermi energy centered around the M point [Fig. 3(c)]. This kink is identical to the

one obtained with the DCA in Ref. [26]. In addition, our results show an additional "splitting" of the bands below and above the Fermi energy along the $k_y = 0$ line and centered at around the X point. The splitting of the bands is accompanied by an additional kink at the Fermi surface. This kink appears at the onset of a branch of excitations that could be traced back to the upper branch of the spinon-antiholon continuum in the one-dimensional Hubbard model [33,35]. Remarkably, these features also appear in DCA calculations [56] which in principle should not have any "memory" of 1D physics and spin-charge separation. The splitting, though it is more marked in our results, can be interpreted as a pseudogap, as we can clearly see in a cut along the frequency axes in Fig. 3(c), in agreement with previous observations. We point out, however, that CPT calculations on 4×4 clusters [35] show instead a flat dispersion, similar to the one observed in the undoped case. Although in Ref. [35] it is identified as a pseudogap, it is not sufficiently resolved due to the small system size.

IV. DISCUSSION

We have presented a study of the spectral properties of the 2D Hubbard model using the DMRG method as a cluster solver for CPT. Our clusters are "infinite" (very long) two-leg ladders, which already contain information about the thermodynamic limit along the leg direction. In addition, it is reasonable to expect that due to the large size of the ladders, charge fluctuations inside the clusters are largely reduced. Results show a remarkable resolution of the bands and allow us to identify features such as waterfalls, kinks, and pseudogap, of significance in the physics of cuprate superconductors. We relate these aspects to one-dimensional physics that survives, even in the presence of AFM correlations. We point out that these features are also observed in simulations on 2D clusters, and DCA, indicating that they likely are not artifacts of our cluster choice, despite its breaking rotational symmetry.

Therefore, the main question one should ask is: What is the fate of spin and charge separation in the presence of long-range antiferromagnetic correlations? Whether our spectra display genuine aspects of the physics of the 2D Hubbard model cannot be determined with complete certainty from our results since cluster perturbation theory does not account for the presence of long-range antiferromagnetic order in two dimensions. Ladders are gapped quasi-1D systems, with a fast decay of the correlations (Hubbard ladders have a spin correlation length of about four lattice spacings [71] for $U = 8$ at half-filling). The spin gap and the correlation length decay quite rapidly upon doping. In 2D, long-range AMF order is also expected to be greatly suppressed away from half-filling. The remarkable agreement with Monte Carlo [10,11,15,16], VCA [22,25], and DCA [26] on square clusters, indicates that our ladders contain a great deal of information and display features corresponding to the 2D physics of the Hubbard model. In addition, 2D-AFM long-range order exists only at zero temperature, so it is conceivable that the CPT spectrum is a faithful representation of the excitations of the system at finite T, after the correlation length reduces to a few lattice spacings, as also suggested by the aforementioned QMC results [16]. Further studies to elucidate these questions may have to consider the artificial addition of a staggered magnetic field *à la* VCA.

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