Spectral weight function for the two-dimensional Hubbard model

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We present results for the single-particle spectral weight function for the two-dimensional Hubbard model. Results were obtained using analytic expressions for the first two moments of the spectral weight function, along with numerical calculations using a combination of quantum Monte Carlo and the maximum-entropy method of analytic continuation. The expressions for the first two moments are surprisingly simple, involving only the parameters of the model, the chemical potential, and the filling. At half-filling, the squared width (variance) of the spectral weight is exactly $U^2/4$. Numerical results are shown for 8×8 lattices at a variety of fillings and momenta. The insulating antiferromagnetic gap in the spectral weights, readily apparent in the results at half-filling, is absent at a filling of 0.95.

Because of its relevance to high temperature superconductivity, the two-dimensional (2D) Hubbard model has received a substantial amount of attention from theorists in recent years. Despite this, relatively little is known about some of its properties, including the single-particle spectral weight function. In this paper we present analytic and numerical results for the spectral weight function. The analytic results are in the form of moments of the spectral weight function, and are valid for the model in any dimension and also in the presence of additional hopping terms. The numerical results were produced for 8×8 lattices using a combination of quantum Monte Carlo, the maximum entropy method, and the analytic moments. A complementary approach to the methods used here is the exact diagonalization technique,[1] which has been used to calculate the spectral weight on lattices with as many as 10 sites, but which has unlimited resolution.

In the Lehmann representation, the spectral weight function is given by

$$A(p,\omega)=\frac{1}{Z}\sum_{s,s'}e^{-\beta E_s}(1+e^{-\beta\omega})|\langle s|c_{p,\uparrow}|s'\rangle|^2\delta(\omega-(E_{s'}-E_s)) , \tag{1}$$

where Z is the partition function and s and s' are complete sets of many-particle eigenstates. The moments μ_m of $A(p,\omega)$ are defined through

$$\mu_m=\int_{-\infty}^{\infty}d\omega\,\omega^m A(p,\omega) . \tag{2}$$

Note that $\mu_0=1$. From (1) one can show that[2]

$$\mu_m=\langle\{[c_{p,\uparrow},H]_m,c_{p,\uparrow}^{\dagger}\}\rangle , \tag{3}$$

where $\{,\}$ denotes an anticommutator, H is the Hamiltonian, and $[,]_m$ is a multiple (nested) commutator, with $[a,b]_1\equiv[a,b]$, $[a,b]_2\equiv[[a,b],b]$, etc. The Hamiltonian in momentum space is

$$H=\sum_{p,\sigma}(\varepsilon_p-\mu)c_{p,\sigma}^{\dagger}c_{p,\sigma}+\frac{U}{N}\sum_{k,p,q}c_{p+q,\uparrow}^{\dagger}c_{k-q,\downarrow}^{\dagger}c_{k,\downarrow}c_{p,\uparrow} , \tag{4}$$

where (in 2D) $\varepsilon_p=-2t(\cos p_x+\cos p_y)$, the lattice spacing is taken to be 1, and N is the number of sites.

Evaluation of the commutators for the first two moments gives

$$\mu_1=\varepsilon_p-\mu+\langle n\rangle U/2 \tag{5}$$

and

$$\mu_2=(\varepsilon_p-\mu)^2+U(\varepsilon_p-\mu)\langle n\rangle+\tfrac{1}{2}U^2\langle n\rangle , \tag{6}$$

where $\langle n\rangle$ is the filling. In evaluating these expressions, no use was made of the specified form of ε_p, so the relations hold in the presence of additional next-nearest-neighbor hopping, dimensions other than two, etc. The results are also valid at any temperature. The results are surprisingly simple for the second moment: no two-particle correlation functions need to be evaluated. For general fillings, one must evaluate $\langle n\rangle$ as a function of μ numerically (which can usually be done quite accurately), but $\mu=U/2$ corresponds exactly to half-filling, $\langle n\rangle=1$. In that case, $\mu_1=\varepsilon_p$ and $\mu_2=U^2/4+\varepsilon_p^2$. The squared width (variance) of the spectral weight is given by $\mu_2-\mu_1^2$, and in the case of half-filling is exactly $U^2/4$. These expressions have been checked with results from an exact diagonalization of a 2×2 lattice; perfect agreement was found.

We have also obtained the expression for the third mo-

ment. It involves two-particle correlation functions, which could be evaluated with Monte Carlo methods, and in principle higher moments could be obtained as well. However, the difficulty in calculating the commutators as well as the difficulty in calculating the required correlation functions make the reconstruction of the spectral weight using only the moments impractical. We use only the first and second moments here.[3]

Information about $A(p,\omega)$ is also contained in the finite-temperature, imaginary-time Green's function

$$G(p,\tau)\equiv -\langle \mathcal{T}_\tau[c_{p,\uparrow}(\tau)c^\dagger_{p,\uparrow}(0)]\rangle \tag{7}$$

through the relation

$$G(p,\tau>0)=-\int_{-\infty}^{\infty} d\omega \frac{A(p,\omega)e^{-\tau\omega}}{1+e^{-\beta\omega}} . \tag{8}$$

It has become fairly straightforward now to calculate $G(p,\tau)$ using quantum Monte Carlo methods.[4,5] Recent work in numerical analytic continuation has addressed the problem of inverting (8) to find $A(p,\omega)$ for $G(p,\tau)$. This problem is equivalent to doing a numerical inverse Laplace transform, which is known to be highly unstable. The problem is made even more difficult here by the presence of statistical errors in the Monte Carlo data for $G(p,\tau)$. Nevertheless, several reasonable ways now exist to analytically continue $G(p,\tau)$ to obtain the spectral weight.[6-9] For this work we have chosen the maximum entropy method.[8]

The quantum Monte Carlo calculations we use are formulated using a Hubbard-Stratonovich transformation to cast the problem in single particle form, and use matrix factorization techniques to reach low temperatures.[5,10] The calculations yield $G(p,\tau)$ at a discrete set of τ points $\tau_l = l\,\Delta\tau$, $l=0,1,\ldots,L$, with $L\,\Delta\tau=\beta$. One can also associate a statistical error σ_l with each point; however, the statistical errors for different values of τ_l will in general be quite correlated. We therefore describe the statistical errors in terms of the full covariance matrix $C_{l,l'}$.[8] Note that $C_{l,l}=\sigma_l^2$.

If one has a proposed spectral weight function, then one can compare this spectrum to the data by transforming it via (8), obtaining a proposed Green's function $\bar{G}(p,\tau_l)$. One can then calculate the χ^2 fit of the function to the data $G(p,\tau_l)$ using the inverse of the covariance matrix via

$$\chi^2=\sum_{l,l'}\delta_l[C^{-1}]_{l,l'}\delta_{l'} , \tag{9}$$

where

$$\delta_l\equiv G(p,\tau_l)-\bar{G}(p,\tau_l) . \tag{10}$$

A overly simple way to calculate the spectral weight is to vary $A(p,\omega)$ to get a minimum of χ^2, subject to the constraint $A(p,\omega)\geq 0$. This approach ignores the instability inherent in the problem, and gives very poor results, characterized by excessive amounts of structure in the results where none is warranted by the data. Other recently developed, more successful approaches minimize the sum of χ^2 and an additional term which penalizes spectra which have excessive structure. In the maximum-entropy method, one seeks to maximize

$$-\tfrac{1}{2}\chi^2+\alpha\int d\omega\left[A(p,\omega)-m(\omega)-A(p,\omega)\ln\left[\frac{A(p,\omega)}{m(\omega)}\right]\right] . \tag{11}$$

The second term is proportional to the entropy of the spectrum relative to a default model $m(\omega)$. This term penalizes deviations of $A(p,\omega)$ from $m(\omega)$, thus reducing excessive structure. The parameter α is set using probability arguments to provide a proper balance between fitting the data and not fitting the *statistical errors* in the data.[8]

A natural way to choose the default model $m(\omega)$ is by variationally maximizing the entropy functional $-\int d\omega\, m(\omega)\ln m(\omega)$ subject to the constraint that the moments μ_0, μ_1, and μ_2 be given correctly.[11] This yields a Gaussian of the form

$$m(\omega)=[2\pi(\mu_2-\mu_1^2)]^{-1/2}\exp[-\tfrac{1}{2}(\omega-\mu_1)^2/(\mu_2-\mu_1^2)] . \tag{12}$$

However, we have found the actual spectral weights to have much more weight in the tails than is given by (12). It is much better to have a default model which is too broad, rather than too narrow: a broad model simply

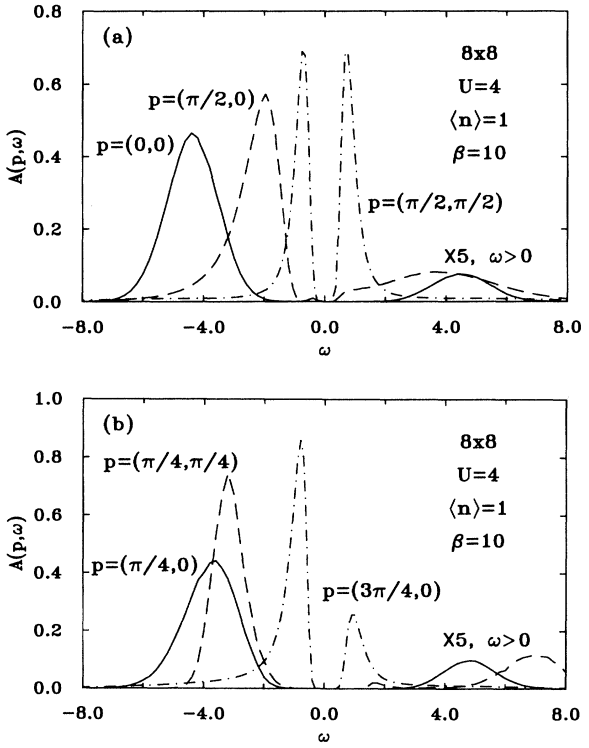

FIG. 1. Spectral weight function at half-filling. The parts of the curves with $\omega>0$ for the momenta $p=(0,0)$, $(\pi/4,0)$, $(\pi/2,0)$, and $(\pi/4,\pi/4)$ have been multiplied by 5 to show detail.

fails to provide much information to the fitting procedure, whereas an overly narrow model artificially cuts off the tails. Therefore, in the results shown here we have used a default model with width $2(\mu_2-\mu_1^2)^{1/2}$ instead of $(\mu_2-\mu_1^2)^{1/2}$. [The results were insensitive to the precise width of $m(\omega)$.] Instead of imposing the correct moments through the default model, we incorporated them in the form of a modified χ^2. We use

$$\chi'^2=\chi^2+\frac{1}{\sigma^2}\sum_{m=1}^{2}\left[\mu_m-\int d\omega\,\omega^m A(p,\omega)\right]^2, \quad (13)$$

with $\sigma=0.1$ for the results shown here. This ensures that the moments in the resulting spectra are accurate to within two or three σ.

In interpreting the spectra it is useful to think of the analytic continuation procedure as being similar to a finite resolution spectrometer which broadens the spectra by some width $\Delta\omega$. The cause of the finite resolution is the statistical errors in the Monte Carlo data. In this case, however, $\Delta\omega$ varies with ω. It is smallest near $\omega=0$. Use of the moments helps reduce $\Delta\omega$ for larger ω, but only to a limited extent. Unfortunately, it is difficult to make these somewhat general statements about $\Delta\omega$ more specific, since at this point we lack even a rigorous definition of $\Delta\omega$. A procedure giving a rough estimate[12] of $\Delta\omega$ indicates that the width of the main peak in each of the spectra shown here should be taken as an estimate of $\Delta\omega$, and *an upper bound* to the true width, rather than as *an estimate* of the true width. The data for the most part is not accurate enough to resolve the true widths.

Figure 1 shows results for half-filling at a fairly low temperature, $\beta=10$, for a variety of wave vectors, on an 8×8 lattice.[13] (All energies are in units of the hopping t.) The noninteracting Fermi surface is a tilted square, with $p=(\pi/2,\pi/2)$ at the center of a side, and $p=(\pi,0)$ at a corner. The antiferromagnetic gap shows itself as a splitting of the central peak for the wave vector $p=(\pi/2,\pi/2)$. Our results for the other wave vectors on the noninteracting Fermi surface are identical (within statistical errors) to those for $p=(\pi/2,\pi/2)$.

Figure 2 shows results for a filling 0.95. At this filling the quantum Monte Carlo method cannot reach low temperatures because of fermion sign problems.[14] Here we show results for $\beta=5$. At this filling we do not see any sign of an antiferromagnetic gap for wave vectors near the Fermi surface. In fact, for both $p=(\pi,0)$ and $p=(\pi/2,\pi/2)$, the main peak occurs at $\omega=0$, although the first moment is not zero ($\mu_1=0.35$ for each). The moment is satisfied by asymmetrical tails. The slight difference between the spectra for $p=(\pi,0)$ and $p=(\pi/2,\pi/2)$ is statistically significant.

Figure 3 shows results for a filling of 0.87 and $\beta=5$. The results are similar to the $\langle n\rangle=0.95$ case. However, the spectra have less weight in the tails for wave vectors near the Fermi surface. The peaks also appear sharper near $\omega=0$, although the statistical significance of this is difficult to judge. Now the peak for $p=(\pi/2,\pi/2)$ is

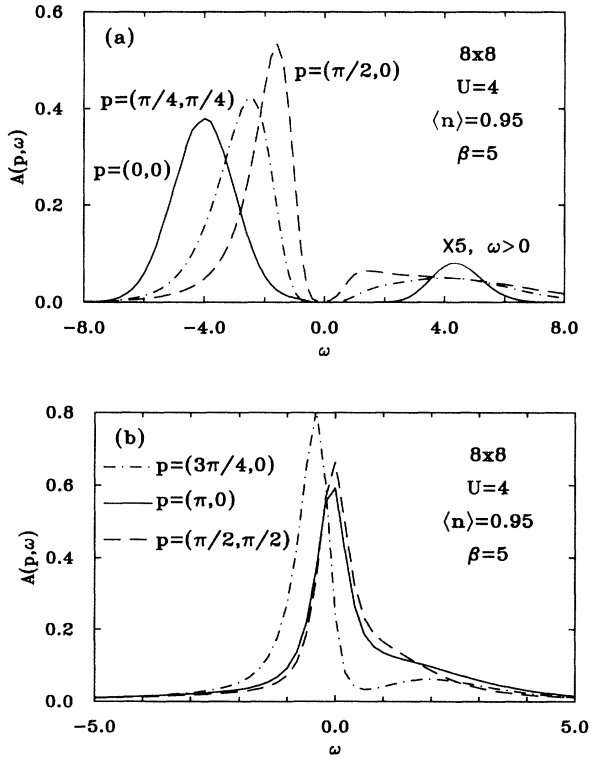

FIG. 2. Spectral weight function at a filling 0.95. The parts of the curves with $\omega>0$ in (a) have been multiplied by 5 to show detail.

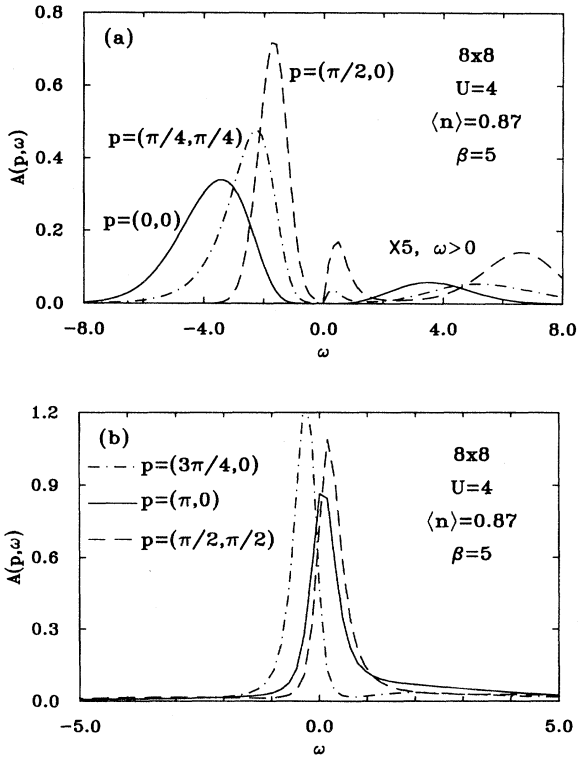

FIG. 3. Spectral weight function at a filling of 0.87. The parts of the curves with $\omega>0$ in (a) have been multiplied by 5 to show detail.

definitely shifted to the right of the peak for $p=(\pi,0)$. This is consistent with the Monte Carlo results for the momentum occupation, $\langle n_p \rangle = 0.28$ at $p=(\pi/2,\pi/2)$ and $\langle n_p \rangle = 0.33$ at $p=(\pi,0)$.

Our work has revealed many of the main features of the spectral weight function for several fillings. These results should be useful as constraints on theoretical approaches to the model. The analytic results in particular will be very useful as checks on numerical or approximate calculations. For some specific details, however, such as the behavior of $A(p,\omega)$ at very low temperatures away from half-filling, we will have to wait for more powerful techniques.

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[2]This result must be well known, but we have not found a reference for it.

[3]We have also not used moments of the form $\bar{\mu}_m \equiv \int d\omega\, \omega^m A(p,\omega)/(e^{\beta\omega}+1)$. We find $\bar{\mu}_m = \langle c^\dagger_{p,\uparrow} [c_{p,\uparrow}, H]_m \rangle$. Knowing $\bar{\mu}_0$ is equivalent to knowing $G(p,\tau=0)$.

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[11]R. N. Silver, private communication.

[12]S. R. White, unpublished.

[13]Recent work by White, Scalapino, Sugar, and Bickers (Ref. 6) showed results for $p=(\pi/2,\pi/2)$ which had all of the spectral weight for $|\omega|>2$ concentrated in two "satellite" peaks at $\omega=\pm 4$, as opposed to the smooth tails shown here. We now believe that those peaks were artifacts of the analytic continuation method used there.

[14]E. Y. Loh, J. E. Gubernatis, R. T. Scalettar, S. R. White, D. J. Scalapino, and R. L. Sugar, Phys. Rev. B **41**, 9301 (1990).