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Pseudogap formation in the half-filled Hubbard model

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Using quantum Monte Carlo, we study the evolution of pseudogaps in the spectral weight function for a half-filled two-dimensional Hubbard model as a function of temperature and coupling constant. The formation of pseudogaps at finite temperature can be used to distinguish between three regimes: (1) a strong-coupling Mott-Hubbard regime, characterized by a pseudogap which persists even at high temperatures; (2) a weak-coupling spin-density-wave regime, characterized by the absence of a pseudogap at any finite temperature; and (3) an intermediate-coupling regime with mixed behavior, characterized by a pseudogap that appears at a finite temperature.

In both the weak- and strong-coupling limits, the two-dimensional (2D) Hubbard model has an insulating antiferromagnetic gap in the single-particle density of states at half-filling and zero temperature. Despite this similarity, and the corresponding absence of a metal-insulator transition, the two limits are quite different. In weak coupling ($U \ll W$, where the bandwidth $W=8t$) the gap Δ results from a spin-density-wave (SDW) instability, related to the presence of both a Van Hove singularity and perfect nesting of the Fermi surface, and varies as $\Delta \approx te^{-2\pi\sqrt{t/U}}$. In strong coupling ($U \gg W$) the gap is described in the Mott-Hubbard picture as resulting from the large energy cost of creating a doubly occupied site, and varies as $\Delta \approx U$. It appears that the gap smoothly interpolates between the two regimes. It would be useful to be able to calculate some property of the system which would better characterize whether the system is in the SDW or the Mott-Hubbard regime for intermediate values of U/t. We believe that the behavior of pseudogaps at finite temperature provides such a means. In fact, by studying pseudogap formation using quantum Monte Carlo, we have identified three regimes: (1) a strong-coupling Mott-Hubbard regime, characterized by a pseudogap which persists even at high temperatures; (2) a weak-coupling spin-density-wave regime, characterized by the absence of a pseudogap at any finite temperature; and (3) an intermediate-coupling regime with mixed behavior, characterized by a pseudogap that appears at finite T.

We emphasize that these are not distinct phases, only different regimes, with smooth transitions between them, as characterized by the behavior of the spectral weight function. Since the presence or absence of a gap or pseudogap is of fundamental importance in determining the properties of a system, we believe that this type of characterization is useful.

We consider the positive-U Hubbard Hamiltonian[1]

$$H=-t\sum_{\langle i,j\rangle,\sigma}(c_{i\sigma}^{\dagger}c_{j\sigma}+c_{j\sigma}^{\dagger}c_{i\sigma})+U\sum_{i}n_{i\uparrow}n_{i\downarrow}-\mu\sum_{i,\sigma}n_{i\sigma}\ , \tag{1}$$

on a two-dimensional lattice, which consists of a system of electrons with an on-site interaction with coupling constant U. Here t is the nearest-neighbor hopping parameter (we have set $t=1$ throughout), and μ is the chemical potential, with $\mu=U/2$ at half-filling. The $c_{i\sigma}^{\dagger}$ are fermion creation operators at site i with spin σ, and $n_{i\sigma}=c_{i\sigma}^{\dagger}c_{i\sigma}$.

The weak-coupling regime has been extensively studied within perturbation theory,[2] mean-field approximations,[3] and quantum Monte Carlo techniques,[4] confirming a phase transition to an antiferromagnetic insulator at $T=0$ in accordance with the Mermin-Wagner theorem.[5] The Mott-Hubbard regime has been previously examined in strong-coupling expansion,[6–8] in which case, to lowest order in t/U, the half-filled system maps into the Heisenberg model with $J=4t^2/U$. The $T=0$ behavior has also been solved with exact-diagonalization techniques[9–11] on finite lattices using the Lanczos algorithm.

Our approach[12] consists of using quantum Monte Carlo[13] to find the Matsubara Green's function, $G(p,\tau)$, and then using the maximum entropy method[14,15] to analytically continue to obtain the spectral weight function, $A(p,\omega)$. The maximum entropy method inverts the integral relation

$$G(p,\tau>0)=-\int_{-\infty}^{\infty}d\omega\frac{A(p,\omega)e^{-\tau\omega}}{1+e^{-\beta\omega}}\ . \tag{2}$$

Additional constraints are placed on the analytic continuation via moments[12]

$$\mu_m=\int_{-\infty}^{\infty}d\omega\,\omega^m A(p,\omega)\ . \tag{3}$$

In particular, for p on the noninteracting Fermi surface (with single-particle energy $\epsilon_p=0$), we have $\mu_0=1$, $\mu_1=0$, and $\mu_2=U^2/4$.

Since the analytic continuation procedure used by the maximum entropy method is highly sensitive to the statistical errors of the quantum Monte Carlo Green's function, $G(p,\tau)$, we can only resolve coarse features of the spectral function, $A(p,\omega)$, such as the presence or absence of a pseudogap with width of order t or U. The finer features, such as the sequence of spikes characterizing the spectral function of finite-size systems, or the difference between a full gap and a pseudogap with very

small weight in the gap region, are not resolved. Our discussion of the three regimes do not rely on finer resolution than we can obtain, and we supplement our results for the coarse structure of $A(p,\omega)$ with direct analysis of $G(p,\tau)$.

One of us has previously considered in detail[4] the behavior of pseudogaps at half-filling and finite T for $U=4$, which lies in the weak-coupling regime. Although for any finite lattice a pseudogap appears when the spin-spin correlations reach the size of the system, in the infinite lattice the pseudogap only appears at $T=0$, where the two-dimensional Hubbard model has a phase transition to an antiferromagnetic state. Some of the evidence is presented in Fig. 1, where we show the spectral weight function $A(p,\omega)$ evaluated at $p=(\pi/2,\pi/2)$ for different lattice sizes with $U=4$ and at $\beta=5$. We can clearly conclude that finite-size effects are very important in this case. In order to confirm the behavior of the pseudogap formation from the maximum entropy method, we use an additional method which consists of directly comparing the Matsubara Green's functions at different temperatures. The presence or absence of a gap is most evident in $G(p,\tau)$ near $\tau=\beta/2$; however, some reference is needed to indicate whether a particular value of $G(p,\beta/2)$ corresponds to a gap. We used reference curves for

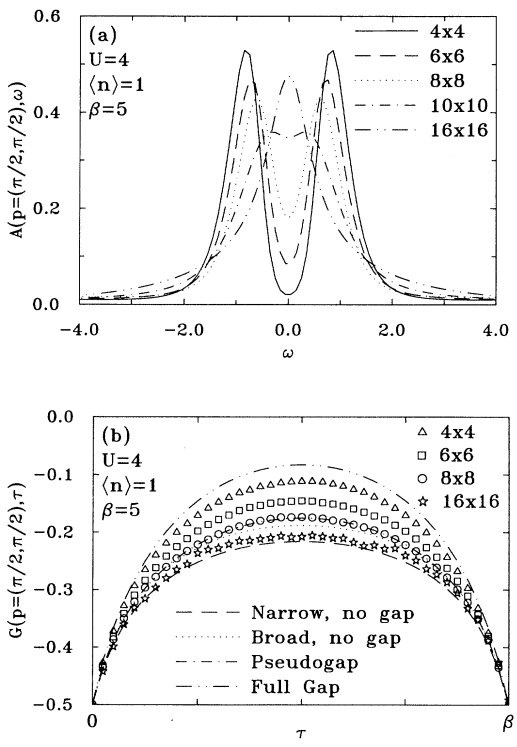

FIG. 1. (a) The spectral weight function $A(p,\omega)$, evaluated at $p=(\pi/2,\pi/2)$ for different lattice sizes for $U=4$ and $\beta=5$. (b) The Matsubara Green's function, $G(p,\tau)$, for $\beta=5$ with $U=4$ for different lattice sizes with reference curves for comparison obtained from a narrow spectrum with no gap (dashed line), a broad spectrum with no gap (dotted line), a pseudogap (dashed-dotted line), and a full gap (dashed-double-dotted line).

$G(p,\tau)$ generated through Eq. (2) from four spectral weight functions: a broad and a narrow Gaussian spectra, and two others with a full gap and a pseudogap at low enough temperatures, all satisfying the correct moments. In Fig. 1(b) we show the Matsubara Green's function at $\beta=5$, with $U=4$ for several lattice sizes with reference curves. This method of comparison proves that this striking finite-size effect is not an artifact of the analytic continuation. Further comparison showed[4] that a pseudogap was present only at temperatures where the antiferromagnetic correlation length was comparable to the size of the system. In the results shown in Fig. 1 the correlation length was about 6 lattice spacings. Since the antiferromagnetic order parameter has a continuous symmetry, from the Mermin and Wagner theorem it is known that the infinite two-dimensional system will only have a phase transition at $T=0$. Hence we conclude that no pseudogap is present at any finite temperature in the infinite system.

In the opposite limit of strong coupling, $U/W\gg 1$, where the Hubbard Hamiltonian maps into the antiferromagnetic Heisenberg model with coupling $J=4t^2/U$, the single-particle density of states, $N(\omega)$, is characterized by two distinct bands with peaks separated by a distance U, which gives us a measure of the gap Δ. The existence of the gap is also present in the spectral weight function, since $N(\omega)=(1/N)\sum_p A(p,\omega)$. In the limit of $t/U=0$, the Mott-Hubbard regime is characterized by a spectral weight function given by

$$A(p,\omega)=\frac{1}{2}\left[\delta\left[\omega-\frac{U}{2}\right]+\delta\left[\omega+\frac{U}{2}\right]\right]. \tag{4}$$

The effect of a finite and small nearest-neighbor hopping is to provide a finite width to the two peaks. In this strong-coupling limit, we have considered the case $U=12$. In Fig. 2 we show the spectral weight function $A(p,\omega)$ evaluated at $p=(\pi/2,\pi/2)$ for several temperatures in the region $t<T<U$, with $U=12$ on a 4×4 lattice. For the temperatures relevant to pseudogap formation in this regime, we have found that no significant finite-size effects are present, which allows us to extend our discussion to the finite system. It is clear that the pseudogap persists at high temperatures, and is thus consistent with the $U/W\gg1$ Mott-Hubbard picture.

In the intermediate-coupling regime we have considered the case $U=8$. In Fig. 3(a) we show the spectral weight function $A(p,\omega)$ evaluated at $p=(\pi/2,\pi/2)$ for different temperatures for $U=8$ on a 4×4 lattice. It is apparent that the gap at $T=1$ gradually develops into a pseudogap at $T=4$ and eventually disappears for $T=8$. Throughout this temperature range spin-spin correlations are short ranged, and no finite-size effects are observed for 4×4 versus larger lattices. However, since the maximum entropy method is highly sensitive to statistical errors in the quantum Monte Carlo data, we have used two additional methods to confirm the behavior of $A(p,\omega)$ in additional to the reference curves method described for weak coupling. The three methods used for determining the pseudogap formation have shown consistent behavior, allowing us to conclude with some assuredness

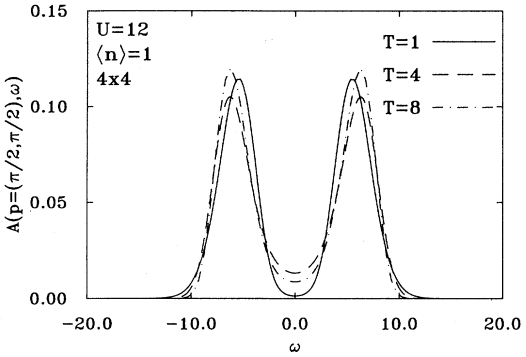

FIG. 2. The spectral weight function $A(p,\omega)$ evaluated at $p=(\pi/2,\pi/2)$ for different temperatures for $U=12$ on a 4×4 lattice.

whether there is or there is not gap formation in the spectral weight function as a function of temperature.

The first method consists of fitting the Monte Carlo data for $G(p,\tau)$ with a trial Green's function derived from Eq. (2) with a one-parameter double-Gaussian function which is properly normalized and has the correct moments, μ_1 and μ_2. In Fig. 3(b) we use this fitting method to show the same qualitative behavior for the development of the gap obtained from the maximum entropy method.

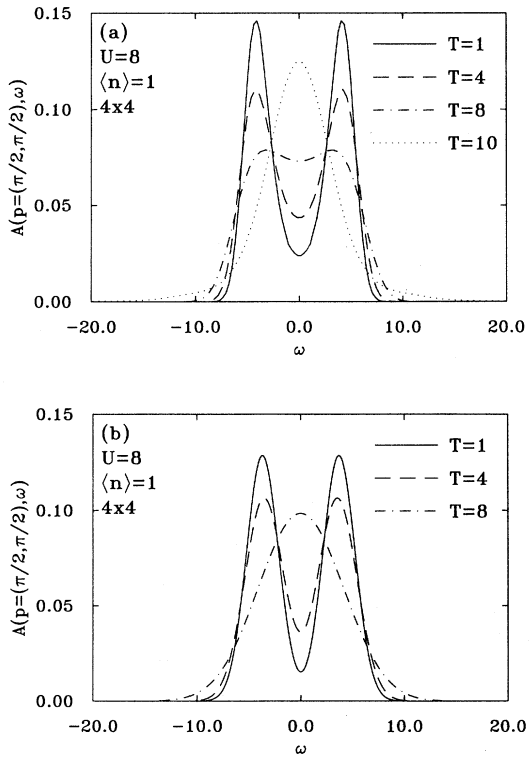

FIG. 3. The spectral weight function $A(p,\omega)$ evaluated at $p=(\pi/2,\pi/2)$ for different temperatures for $U=8$ on a 4×4 lattice. In (a) we use the maximum entropy method, and in (b) we use the double-Gaussian fitting procedure.

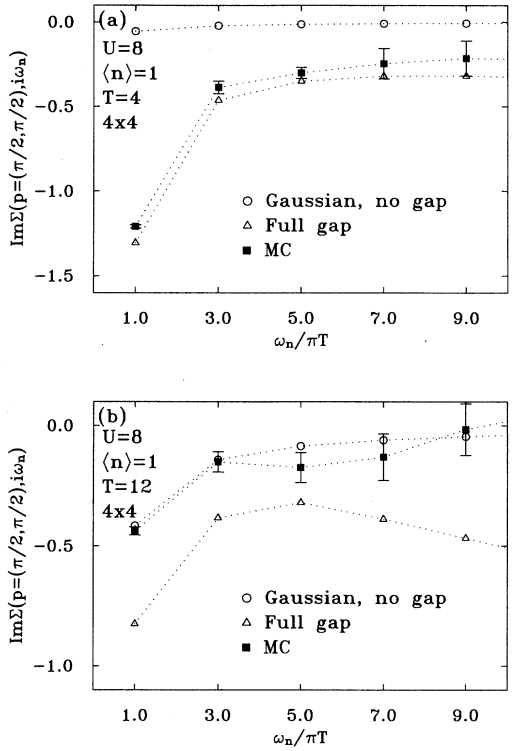

FIG. 4. The imaginary part of the electron self-energy $\mathrm{Im}\Sigma(p,i\omega_n)$ for $U=8$ on a 4×4 lattice. The reference curves for comparison are obtained from a Gaussian spectrum (circles) and from a spectrum with a full gap for $U=6$ and at $\beta=4$ (triangles). In (a) $T=4$, and (b) $T=12$.

The second method consists of looking at the electron self-energy,

$$\Sigma(p,i\omega_n)=-G^{-1}(p,i\omega_n)+i\omega_n+(\epsilon_k-\mu)\ . \tag{5}$$

In general, a divergent quantum Monte Carlo imaginary

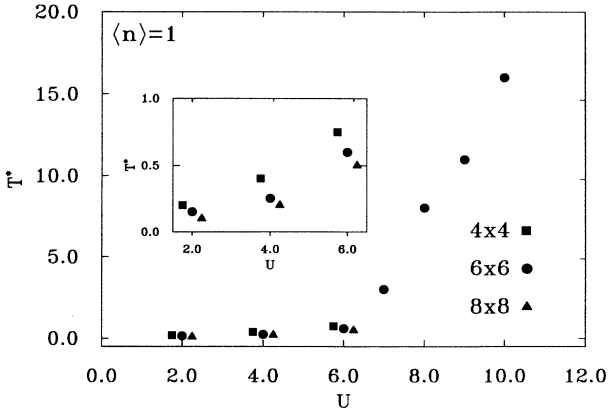

FIG. 5. The temperature T^* at which the gap develops vs U for 4×4, 6×6, and 8×8 lattices.

self-energy at small frequencies implies the presence of a nonvanishing gap. Within mean field theory, if p is on the noninteracting Fermi surface, the imaginary part of the self-energy varies as $-\Delta^2/\omega_n$. In order to determine whether $\mathrm{Im}\Sigma(p,i\omega_n)$ diverges at small frequencies, we must have some sort of reference curves for comparison. We obtained reference curves by taking spectra for $A(p,\omega)$ with clear behavior (either a full gap or no gap), and then using Eq. (2), followed by a Fourier transform, and using Eq. (5). In Fig. 4(a) we plot $\mathrm{Im}\Sigma(p,i\omega_n)$ from the quantum Monte Carlo data for $U=8$ and $T=4$. Since the Monte Carlo $\mathrm{Im}\Sigma(p,i\omega_n)$ behaves very similarly to the reference spectrum with a full gap, we conclude that at $T=4$ the spectral function must have a pseudogap for $U=8$. In Fig. 4(b) we plot $\mathrm{Im}\Sigma(p,i\omega_n)$ at $T=12$. In this case we see that $\mathrm{Im}\Sigma(p,i\omega_n)$ behaves very much like the reference curve with no gap, which leads us to conclude that there is no pseudogap. The behavior of $\mathrm{Im}\Sigma(p,i\omega_n)$ shown in Fig. 4 is clearly different from that of a Fermi liquid, in which case the imaginary part of the self-energy on the Fermi surface exhibits a negative slope for small values of ω_n, and causes a single quasiparticle peak in $A(p,\omega)$ at $\omega=0$.

In Fig. 5 we show a plot of the approximate temperature T^* at which the pseudogap is formed versus U for different lattice sizes. For $U>6$, where there are no finite-size effects, only the 6×6 results are given. We clearly see that a value of $U\approx7$ marks the transition from a region of a pseudogap opening at zero temperature only, in the finite system, to a region where the gap is present at finite temperatures. The value of $U>11$ marks the boundary to the Mott-Hubbard regime, where the gap is always present, even for temperatures of order U. We see that the evolution of the pseudogap clearly distinguishes these three regimes.

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