

Comment on “Absence of a Slater Transition in the Two-Dimensional Hubbard Model”

While we agree with the numerical results of Ref. [1], we arrive at different conclusions: The apparent opening of a gap at finite temperature in the two-dimensional *weak-coupling* Hubbard model at half filling does not necessitate an infinite correlation length ξ (Slater mechanism) nor a thermodynamic *finite-temperature* metal insulator transition (MIT). The pseudogap is a crossover phenomenon due to critical fluctuations in two dimensions, namely, to the effect of a (π, π) spin-density wave (SDW) ξ that is large compared with the thermal length.

We use the units of Ref. [1]. The inset of Fig. 1 shows $\langle n_{\uparrow}n_{\downarrow} \rangle$ obtained in Ref. [1] for $N_c = 36$, $U = 1$ and $N_c = 64$, $U = 0.5$ along with the corresponding results obtained [2] from the local moment sum rule $(T/N_c) \times \sum_q \chi_{\text{sp}}(q) = 1 - 2\langle n_{\uparrow}n_{\downarrow} \rangle$, supplemented with the relations $\chi_{\text{sp}}^{-1}(q) = \chi_0(q)^{-1} - \frac{U_{\text{sp}}}{2}$ and $U_{\text{sp}} = U\langle n_{\uparrow}n_{\downarrow} \rangle / (\langle n_{\uparrow} \rangle \langle n_{\downarrow} \rangle)$. Figure 1 also shows the pseudogap in the density of states $\rho(\omega)$ obtained from [3] $\Sigma_{\sigma}^{(s)}(k) = Un_{-\sigma} + \frac{U}{8} \frac{1}{N} \sum_q [3U_{\text{sp}}\chi_{\text{sp}}(q) + U_{\text{ch}}\chi_{\text{ch}}(q)]G_{\sigma}^0(k+q)$ which includes the effects of both spin χ_{sp} and charge χ_{ch} fluctuations and satisfies $\frac{1}{2}\text{Tr}[\Sigma_{\sigma}^{(s)}G_{\sigma}^0] = U\langle n_{\uparrow}n_{\downarrow} \rangle$. The charge fluctuations are constrained by the sum rule $(T/N_c) \sum_q [\chi_{\text{sp}}(q) + \chi_{\text{ch}}(q)] = 1$. As temperature is lowered from $T = 1/20$ to $1/22$ and $1/32$, the pseudogap in $\rho(\omega)$ quickly deepens. The distance between the two peaks is in quantitative agreement with Ref. [1]. In addition, extensive comparisons with quantum Monte Carlo (QMC) have shown earlier [2,3] that our approach agrees quantitatively with QMC, and contains the same finite-size effects. In particular, $\rho(\omega = 0)$ is smaller in smaller lattices. Hence, while at $T = 1/32$ the criterion [1]

$\rho(\omega = 0) < 1 \times 10^{-2}$ is satisfied for $N_c = 64$ and short $\xi \approx N_c^{1/2}$, we still need to verify that this reflects the behavior of a large (but not infinite) correlation length in the thermodynamic limit. That is why we verified that $\rho(\omega = 0) < 1 \times 10^{-2}$ for $N_c = 128^2$ as well. $\rho(\omega = 0)$ in dynamical cluster approximation (DCA) has the opposite size dependence and satisfies $\rho(\omega = 0) < 1 \times 10^{-2}$ for $N_c = 64$. Note that for size 128^2 , ξ already reaches 40 lattice spacings at $T = 1/22$. All of the above results may be understood analytically from the above equations [2] by considering the limiting case where the characteristic frequency in the spin spectral weight χ_{sp}'' becomes smaller than temperature (renormalized classical regime). The local moment sum rule prevents a finite-temperature mean-field transition by letting U_{sp} , and hence $\langle n_{\uparrow}n_{\downarrow} \rangle$, exhibit a downturn at T^* . Below that temperature, ξ grows rapidly but it becomes infinite only at $T = 0$. Similarly, the opening of the pseudogap with decreasing temperature can be traced [2], in $d = 2$, to the singular contribution of $\chi_{\text{sp}}(q)$ to $\Sigma_{\sigma}^{(s)}(k)$ when ξ becomes larger than the single-particle thermal de Broglie wavelength $\xi_{\text{th}} = v_F/T$. Indeed, in that limit, the single-particle spectral weight $A(\mathbf{k}_H, \omega)$ at hot spots is given by $-2\Sigma''[(\omega - \Sigma')^2 + \Sigma'^2]^{-1}$ with $\omega - \Sigma' = 0$ and $\Sigma''(\mathbf{k}_H, 0) \propto \xi^{3-d}/\xi_{\text{th}}$. Since ξ/ξ_{th} grows exponentially in the $d = 2$ renormalized classical regime, $A(\mathbf{k}_H, \omega)$ can become exponentially small at $\omega = 0$ even without a MIT. In the analytical approach [2], the downturn in $\langle n_{\uparrow}n_{\downarrow} \rangle$ and the opening of a deep pseudogap are both unambiguously driven by a rapidly growing ξ in the SDW channel. The pseudogap is not needed to reinforce the downturn in $\langle n_{\uparrow}n_{\downarrow} \rangle$. While the situation is more subtle than that of Slater, the peaks in Fig. 1 are precursors of the SDW insulator that appears at exactly $T = 0$ by the Slater mechanism. The peak separation in frequency (the gap) is larger than T^* because Kanamori screening strongly renormalizes T^* down.

Increasing N_c in DCA effectively lowers the dimension towards $d = 2$, revealing the effect of $\xi > \xi_{\text{th}}$ on Σ and ρ .

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[1] S. Moukouri and M. Jarrell, Phys. Rev. Lett. **87**, 167010 (2001).

[2] Y. M. Vilk *et al.*, J. Phys. I (France) **7**, 1309 (1997).

[3] S. Moukouri *et al.*, Phys. Rev. B **61**, 7887 (2000).

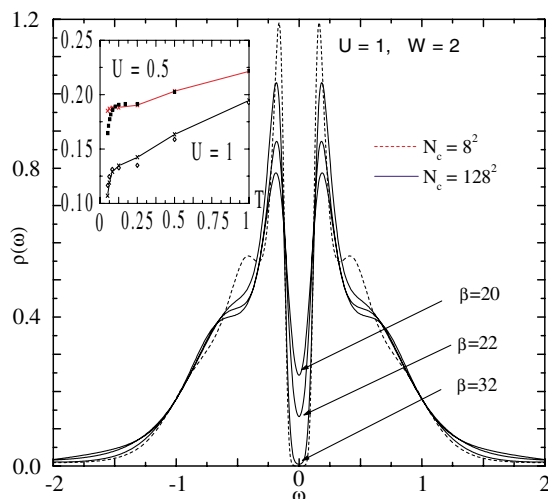


FIG. 1 (color online). Density of states as a function of ω for various lattice sizes, the largest β having the largest peak heights. Inset shows $\langle n_{\uparrow}n_{\downarrow} \rangle$ with symbols from Ref. [1], except for \times and lines that represent our calculation.