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 $\xi$ (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 $(\pi, \pi)$ spin-density wave (SDW) $\xi$ that is large compared with the thermal length. We use the units of Ref. [1]. The inset of Fig. 1 shows $\langle n_1 n_1 \rangle$ 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 $(T/N_c) \sum_\sigma \chi_\sigma(q) = 1 - 2\langle n_1 n_1 \rangle$, supplemented with the relations $\chi_\sigma^{-1}(q) = \chi_0(q)^{-1} - U_\text{sp}$ and $U_\text{sp} = U \langle n_1 n_1 \rangle / \langle (n_1)(n_1) \rangle$. Figure 1 also shows the pseudogap in the density of states $\rho(\omega)$ obtained from [3] $\sum \rho(k) = U n_{-\sigma} + \left( \frac{T}{\pi} \sum_q \rho(q) \right)$ which includes the effects of both spin $\chi_\sigma$ and charge $\chi_{\text{ch}}$ fluctuations and satisfies $\frac{1}{2} \text{Tr}[\Sigma^{(s)} \chi_{\sigma}^\dagger] = U \langle n_1 n_1 \rangle$. The charge fluctuations are constrained by the sum rule $(T/N_c) \sum_q \chi_{\text{ch}}(q) = 1$. 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 $N_c = 128$ 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 $128^2$, $\xi$ 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 $\chi_\sigma^\dagger$ becomes smaller than temperature (renormalized classical regime). The local moment sum rule prevents a finite-temperature mean-field transition by letting $U_\text{sp}$, and hence $\langle n_1 n_1 \rangle$, exhibit a downturn at $T^*$. Below that temperature, $\xi$ 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 $\chi_\sigma$ to $\Sigma^{(s)}(k)$ when $\xi$ 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 $A(k_H, \omega)$ at hot spots is given by $-2\Sigma^{(s)}[(\omega - \Sigma)^2 + \Sigma^{(s)}]^{-1}$ with $\omega > \Sigma = 0$ and $\Sigma^{(s)}(k_H, 0) \propto \xi^{3-d} / \xi_{\text{th}}$. Since $\xi / \xi_{\text{th}}$ grows exponentially in the $d = 2$ renormalized classical regime, $A(k_H, \omega)$ can become exponentially small at $\omega = 0$ even without a MIT. In the analytical approach [2], the downturn in $\langle n_1 n_1 \rangle$ and the opening of a deep pseudogap are both unambiguously driven by a rapidly growing $\xi$ in the SDW channel. The pseudogap is not needed to reinforce the downturn in $\langle n_1 n_1 \rangle$. 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 $\Sigma$ and $\rho$.

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B. Kyung, J. S. Landry, D. Poulin, and A.-M. S. Tremblay* Département de Physique and Centre de Recherche sur les propriétés électroniques de matériaux avancés Université de Sherbrooke, Sherbrooke Quebec, Canada J1K 2R1

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*Electronic address: tremblay@physique.usherbro.ca

