Comment on "Absence of Spin Liquid in Nonfrustrated Correlated Systems"

In a recent Letter, Hassan and Sénéchal [1] discussed the existence of a spin-liquid phase of the half-filled Hubbard model on a honeycomb lattice. Using schemes such as the variational cluster approximation and cluster dynamical mean field theory (CDMFT) in combination with exact diagonalization (ED), they argued that a single bath orbital per site of the six-atom unit cell is insufficient and leads to the erroneous conclusion that the system is gapped for all nonzero values of the Coulomb interaction U. In contrast, we point out that in the case of the honeycomb lattice, six bath levels per six-site unit cell are perfectly adequate for the description of short-range correlations. Instead, we demonstrate that it is the topology of the ring unit cell, combined with the lack of translation symmetry inherent in CDMFT, which opens a gap at Dirac points. The gap found at small U therefore does not correspond to a Mott gap. As a result, the present CDMFT-like schemes for this cell are not suitable for the identification of a spin-liquid phase on a honeycomb lattice.

As shown in Ref. [2], the cluster self-energy obtained in ED CDMFT [3] using six bath levels is in nearly quantitative agreement with results derived in continuous-time quantum Monte Carlo (QMC) CDMFT [4]. As the bath in QMC calculations is infinite, the self-energy is not subject to finite-size effects. The reason for this agreement is that because of the semimetallic nature of the honeycomb lattice, the projection of the bath Green's function on a finite cluster is not plagued by the low-energy disparities that arise in correlated metals. Moreover, because of the hexagonal symmetry, this projection can be performed in the diagonal molecular-orbital basis with nonsymmetric density of states components [3]. The issue raised in Ref. [1] concerning the symmetry of bath levels then does not arise, and the two independent bath Green's function components are fitted accurately using a total of six parameters (see Fig. 24 of [2]).

The self-energy at Dirac points K for the ring unit cell exhibits low-energy behavior [3]: $\Sigma(K, i\omega_n) \approx a i\omega_n + b^2/[i\omega_n(1-a)]$, where $a = \mathrm{Im}[\Sigma_{11}(i\omega_n) - \Sigma_{13}(i\omega_n)]/\omega_n$ and $b = \mathrm{Re}[\Sigma_{12}(i\omega_n) - \Sigma_{14}(i\omega_n)]$ for $\omega_n \to 0$. Σ_{ij} is the self-energy in the site basis, and ω_n are Matsubara frequencies. The gap at low temperatures T is given by $\Delta \approx 2|b|/\sqrt{1-a}$ (see also Ref. [5]). Using the site notation $\mathbf{a}_1 = (0, 0)$, $\mathbf{a}_2 = (0, 1)$, $\mathbf{a}_3 = (\sqrt{3}/2, 3/2)$, $\mathbf{a}_4 = (\sqrt{3}, 1)$, $\mathbf{a}_5 = (\sqrt{3}, 0)$, and $\mathbf{a}_6 = (\sqrt{3}/2, -1/2)$, Σ_{12} and Σ_{14} are independent, so that $\Delta \neq 0$. However, site 1 is also connected to site 4 at $(-\sqrt{3}/2, -1/2)$ in the neighboring cell, requiring $\Sigma_{12} = \Sigma_{14}$. Therefore, the fact that this condition is not fulfilled in CDMFT is responsible for the insulating contribution $\sim 1/i\omega_n$ to the self-energy at K.

Clearly, this term is not related to the properties of the bath used in ED. In fact, in view of the good agreement with ED, the density of states in QMC CDMFT [4] should also reveal a gap at small U and low T.

One way of overcoming these shortcomings is to combine ED or QMC calculations with the dynamical cluster approximation (DCA) which, in contrast to CDMFT, ensures translation symmetry. Thus, the DCA yields $\Sigma_{12} = \Sigma_{14}$, giving semimetallic rather than insulating behavior at small U [6]. As before, the ED self-energy obtained using six bath levels is in excellent agreement with corresponding results derived within QMC calculations.

For $U \approx 4, \ldots, 5$, ED and QMC CDMFT [3,4] yield gaps which agree remarkably well with the gap derived in large-scale QMC calculations [7]. Evidently, this gap corresponds to a Mott gap due to short-range correlations. The key question, however, as to how the semimetallic phase is recovered at small U cannot be studied adequately within CDMFT using the six-site ring since the gap at small U is an artifact of this unit cell.

In conclusion, ED CDMFT and DCA results for the honeycomb lattice using six bath levels per six-site unit cell are consistent with analogous QMC calculations. Thus, the origin of the gap at small U obtained for CDMFT in ED and QMC translation symmetry implied by CDMFT, using the six-site ring unit cell, is not Mott physics but an artifact of the ring unit cell, combined with the violation of translation symmetry implied by CDMFT. This problem can be avoided, for instance, within ED or QMC DCA. We emphasize, however, that other unit cells, e.g., the two- and four-site cells discussed in Ref. [1], are not affected in the same way by deviations from long-range order.

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