Comment on "Universal Spin-Flip Transition in Itinerant Antiferromagnets"

In a recent Letter [1], it is argued that an itinerant antiferromagnet in an external magnetic field undergoes a spin-flip transition, in marked contrast with the behavior of a localized antiferromagnet: for a weak magnetic field, the magnetization is parallel to the field [Fig. 1(a)], and flips to the perpendicular configuration [Fig. 1(b)] at a critical value of the field. A similar spin-flip transition is predicted to occur as a function of temperature.

In this Comment we show—considering only the zero-temperature case—that the conclusions of Ref. [1] are incorrect. The antiferromagnetic state in the perpendicular configuration has a finite transverse susceptibility: a uniform magnetic field applied perpendicular to the antiferromagnetic magnetization will inevitably induce a uniform magnetization. As a result, the energy of the canted state [Fig. 1(c)] will always be lower than that of the antiferromagnetic state in the perpendicular configuration. The actual ground state of the system should be determined from the free energies of the various phases that are considered (including the normal phase). It is not sufficient, as done in Ref. [1], to find a solution with a finite order parameter and infer the ground state from the amplitude of the magnetization. The canted state—not considered in Ref. [1]—turns out to be the antiferromagnetic ground state of the system up to a critical value of the field where the normal state is restored.

To illustrate these points, we consider the mean-field Hamiltonian of the two-dimensional half-filled repulsive Hubbard model in a uniform field H parallel to the z axis and coupled to the fermion spins [2]:

$$H = -\sum_{\mathbf{r},\mathbf{r}'} c_{\mathbf{r}}^{\dagger} t_{\mathbf{r},\mathbf{r}'} c_{\mathbf{r}'} - \sum_{\mathbf{r}} c_{\mathbf{r}}^{\dagger}(h\sigma^z + m\boldsymbol{\sigma}\cdot\mathbf{n}_{\mathbf{r}})c_{\mathbf{r}} + N\frac{m^2}{U}, \quad (1)$$

where $h = \mu_B H$ and $c_{\mathbf{r}} = (c_{\mathbf{r}\uparrow}, c_{\mathbf{r}\downarrow})^T$. N is the total number of sites, $t_{\mathbf{r},\mathbf{r}'}$ a hopping integral between nearest-neighbor sites, and $\boldsymbol{\sigma} = (\sigma^x, \sigma^y, \sigma^z)$ stands for the Pauli matrices. m and $\mathbf{n}_{\mathbf{r}}$ ($\mathbf{n}_{\mathbf{r}}^2 = 1$) determine the amplitude and the direction of the magnetization, respectively. Although written in real space, the Hamiltonian (1) is similar to that considered in Ref. [1]. For $h = 0$ and $\mathbf{n}_{\mathbf{r}} = (-1)^{\mathbf{r}}\hat{\mathbf{z}}$, it describes the crossover from a Slater ($m \sim te^{-2\pi\sqrt{t/U}}$) to a Mott-Heisenberg ($m \sim U/2$) antiferromagnet as U increases [3].

We consider the three antiferromagnetic states that are schematically depicted in Fig. 1, as well as the normal state [Fig. 1(d)]. Diagonalizing the Hamiltonian (1), we obtain the free energy $F^{(\parallel,\perp)} = m^2/U - \sum_\sigma \int_{\mathbf{k}} E^{(\parallel,\perp)+}_{\mathbf{k}\sigma}/2$, where $E^{(\parallel)\pm}_{\mathbf{k}\sigma} = -\sigma h \pm (\epsilon_{\mathbf{k}}^2 + m^2)^{1/2}$ and $E^{(\perp)\pm}_{\mathbf{k}\sigma} = \pm[(\epsilon_{\mathbf{k}} - \sigma h - \sigma m\cos\theta)^2 + (m\sin\theta)^2]^{1/2}$ are the excitation energies (obtained from the poles of the single-particle Green function) and $\epsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y)$ (assuming a square lattice). The amplitude m of the magnetization is obtained from $\partial F/\partial m = 0$. θ is obtained from $\partial F/\partial\theta = 0$ in the canted state (c), whereas $\theta = \pi/2$ in the antiferromagnetic state (b). In the normal phase, $F_N = m^2/U - \int_{\mathbf{k}} |\epsilon_{\mathbf{k}} - h - m|$.

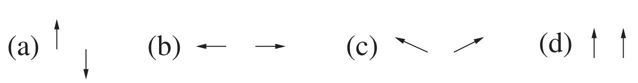

FIG. 1. Antiferromagnetic states: (a) parallel configuration, $\mathbf{n}_{\mathbf{r}} = (-1)^{\mathbf{r}}\hat{\mathbf{z}} \parallel \mathbf{H}$; (b) perpendicular configuration, $\mathbf{n}_{\mathbf{r}} = (-1)^{\mathbf{r}}\hat{\mathbf{x}} \perp \hat{\mathbf{H}}$; (c) canted state, $\mathbf{n}_{\mathbf{r}} = ((-1)^{\mathbf{r}}\sin\theta, 0, \cos\theta)$. (d) The normal state has a ferromagnetic component induced by the magnetic field ($\mathbf{n}_{\mathbf{r}} = \hat{\mathbf{z}}$).

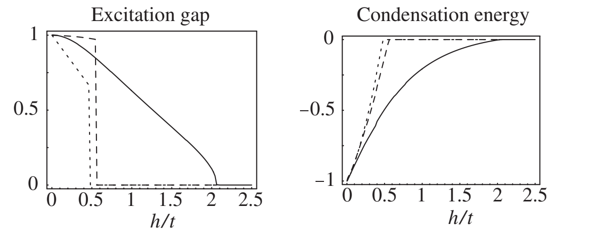

FIG. 2. Left panel: excitation gap in the parallel configuration (a) ($m - h$, short dashed line), the perpendicular configuration (b) (m, long dashed line), and the canted configuration (c) ($m\sin\theta$, solid line) [$U = 4t$]. Right panel: free energy $F^{(\parallel,\perp)} - F_N$. All quantities are normalized to their value at $h = 0$.

For the parallel (a) and perpendicular (b) configurations, the mean-field equation $\partial F/\partial m = 0$ agrees with Ref. [1] and yields the same excitation gap (Fig. 2). Although the parallel configuration has the largest magnetization (m) in weak field [1], it is not the ground state. The free energies are shown in Fig. 2. While the three antiferromagnetic states (a)–(c) are degenerate when $h = 0$, the perpendicular configuration (b) has always a lower free energy than the parallel one (a) for any finite field, in contradiction with the conclusions of Ref. [1]. Moreover, the canted state has the lowest free energy and is therefore the actual ground state. When H increases, the angle θ decreases and vanishes at the second-order phase transition to the normal phase ($h \simeq 2.06t$ in Fig. 2), in qualitative agreement with the behavior of the magnetization in a localized antiferromagnet.

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