Ferromagnetic Spin-Wave Theory in the Multiband Hubbard Model Having a Flat Band

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The peculiar effect of electron correlation in multiband systems is illustrated for the recently proposed ferromagnetism in a Hubbard model having flat bands. Despite the flatness of the band, an acoustic spin-wave mode with a finite stiffness exists along with optical modes below a Stoner gap. The relevant energy (gap and stiffness) transmutes from the Hubbard U in the weak-coupling limit to t (transfer integral) in the strong-coupling limit. This implies a stable itinerant ferromagnetism with finite band widths.

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The correlated electron system in multiband systems having more than one atom per unit cell is interesting, because we expect that the electron repulsion, even when short-ranged (on-site Hubbard U), will exert unusual effects. The correlation effect is in general highlighted by the spin state of the system, which is dominated by the competition between kinetic and interaction energies. Aligned spins have lower interaction energies due to Pauli's principle at the cost of the kinetic energy. In the single-band Hubbard model, however, we can only expect ferromagnetism for $U=\infty$ as in Nagaoka's case of a single hole [1,2].

A drastic effect of the multiband appears in a recent finding of the ferromagnetic ground state in a class of Hubbard systems on decorated lattices that contain flat (dispersionless) bands [3-7]. The appearance of the flat bands is a result of interference of wave functions when we have a certain class of bipartite lattices (Lieb's model) or specially tuned transfer integrals (Mielke or Tasaki's model). In other words, in the flat-band situation, each "Wannier wave function" localized around each unit cell becomes an eigenstate of the tight-binding Hamiltonian. The ground state in each model has been shown to be ferromagnetic with the fully spin-polarized flat band for arbitrary magnitude of $U>0$. Although these models may at first sight seem singular, we can evoke the relevance to real materials. Recently this is done systematically for 2D superstructures conceived for organic materials (π-conjugated electron systems) by Shima and one of the present authors [8].

Now, we think that the discussion of the ground state alone is by far insufficient, and the truly intriguing effect of multibands in such systems should appear in the low-lying excitations (spin waves for a magnetic system): If one regarded the flat band as a heavy-mass limit of an isolated band, one might expect that the dynamics of the spin wave would be singular as well, since the spin stiffness is inversely proportional to the density of state in the single-band model. We shall in fact show here that the multiband correlation effect resumes finite spin stiffness and finite charge gap: In the weak-correlation limit ($U\rightarrow 0$), the k-dependent interaction determines the spectrum, while in the strong-correlation limit ($U\rightarrow\infty$), the exclusion of doubly occupied sites exerts a multiband effect via k-dependent interaction kernels.

The excitation spectrum turns out to comprise an acoustic magnon mode with a finite stiffness along with optical magnon modes below a Stoner (individual charge-excitation) gap that is almost k independent. This holds, surprisingly, for both the weak-correlation and strong-correlation regimes, wherein the energy scale (the gap and the stiffness) transmutes from U to t. The finite stiffness and the gap imply that the ferromagnetism is indeed stable against finite perturbations such as a finite dispersion in the flat band.

We start with the weak-coupling regime. In this limit, there exists the "generalized Hund's coupling" [9] in the Hubbard system, which manifests itself in ferromagnetism in the flat band via the effective exchange interaction [5,9]. To investigate low-lying excitations along this line, we can concentrate on the variation in the spin configuration on the flat band and neglect the interband scattering, which is a higher-order process. This is justified at least when there is a gap between the flat band and other ones as is the case with Tasaki's model [10]. The energy of excited states can then be obtained within the band. The Hamiltonian projected on the flat band (labeled with l) reads in k space

$$\tilde{H}=\sum_{\mathbf{k},\sigma}\varepsilon_l(\mathbf{k})C^\dagger_{l\mathbf{k}\sigma}C_{l\mathbf{k}\sigma}+\sum_{\mathbf{k},\mathbf{p},\mathbf{q}}V(\mathbf{k}+\mathbf{q},\mathbf{p}-\mathbf{q},\mathbf{p},\mathbf{k})C^\dagger_{l\mathbf{k}+\mathbf{q}\uparrow}C^\dagger_{l\mathbf{p}-\mathbf{q}\downarrow}C_{l\mathbf{p}\downarrow}C_{l\mathbf{k}\uparrow}\,, \tag{1}$$

where $C^\dagger_{l\mathbf{k}\sigma}$ creates an electron on the flat band with a wave vector $\mathbf{k}$ and a spin σ.

Since $\varepsilon_l(\mathbf{k})\equiv 0$, all the characteristics of the model are incorporated in the k dependence of the projected coupling constant,

$$V(\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4)=\frac{U}{N_a}\sum_{m=1}^{n}\phi^*_{lm}(\mathbf{k}_1)\phi^*_{lm}(\mathbf{k}_2)\phi_{lm}(\mathbf{k}_3)\phi_{lm}(\mathbf{k}_4)\,, \tag{2}$$

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where the sum is taken for n atoms within a unit cell and $\phi_{lm}(\mathbf{k})$ is the solution of the tight-binding Hamiltonian in the Fourier representation,

$$\sum_{m'} t_{mm'}(\mathbf{k})\phi_{lm'}(\mathbf{k}) = \varepsilon_l(\mathbf{k})\phi_{lm}(\mathbf{k}).$$

This Hamiltonian should generally describe the systems with ferromagnetic ground states as long as the irreducibility of a density matrix on the flat band is fulfilled, which Mielke has shown is a sufficient condition for ferromagnetism [5], and we can show that the condition in turn implies a k-dependent interaction on the flat band.

An excited state with wave vector $\mathbf{q}$ can be obtained as

$$|\chi(\mathbf{q})\rangle = \sum_{\mathbf{k}} f(\mathbf{k}) S^-(\mathbf{k},\mathbf{q})|F\rangle,$$

where $S^-(\mathbf{k},\mathbf{q}) = C^\dagger_{l\mathbf{k}+\mathbf{q}\downarrow} C_{l\mathbf{k}\uparrow}$ flips a spin in the fully polarized flat band, $|F\rangle$. The amplitude $f(\mathbf{k})$ is determined by the usual equation-of-motion method [11] which yields

$$[\hbar\omega_{\mathbf{q}} - \varepsilon_l(\mathbf{k}+\mathbf{q}) + \varepsilon_l(\mathbf{k}) - \Delta_{\mathbf{k}}] f(\mathbf{k}) = -\sum_{\mathbf{p}} V(\mathbf{k}+\mathbf{q},\mathbf{p},\mathbf{k},\mathbf{p}+\mathbf{q}) f(\mathbf{p}), \quad (3)$$

where $\Delta_{\mathbf{k}} = \sum_{\mathbf{p}} V(\mathbf{p},\mathbf{k},\mathbf{k},\mathbf{p})$ is the Stoner excitation gap and $\varepsilon_l(\mathbf{k}) \equiv 0$. We have numerically solved this transcendental equation for typical flat-band models, where a half-filled flat band is fully polarized. The result for Mielke's model [Fig. 1(a)] and for Tasaki's model [Fig. 1(b)] [12] in 2D shows that the low-lying excitations consist of collective modes below a continuum.

In the usual itinerant ferromagnetism with k-independent V, it is the band disperison, $\varepsilon(\mathbf{k})$, that determines the q-dependent magnon dispersion and makes the lower and upper boundaries of the Stoner continuum dispersive. By contrast, since $\varepsilon_l(\mathbf{k}) \equiv 0$ here, the Stoner continuum becomes a rectangular band (with flat top and bottom) whose width equals that of $\Delta_{\mathbf{k}}$ [which coalesces into a line in Mielke's model, Fig. 1(a)]. The spin wave, on the other hand, does have a dispersion with a finite stiffness of order U, which comes from the k dependence of the coupling constant in Eq. (3) [13]. The collective modes comprise a gapless spin wave (acoustic magnon) along with optical one(s) which involve spatial spin oscillations within a unit cell. The number of magnon branches equals the number of $\phi_{lm}(\mathbf{k})$ that is not identically zero.

Mielke and Tasaki have discussed the upper bound for the magnon dispersion by reducing the Coulomb interaction to a spin Hamiltonian on the flat band [7]. They have shown that the spin Hamiltonian in the condition of the local connectivity simplifies into the Heisenberg model for a certain choice of the (nonorthogonal) basis. In the present Hamiltonian, which includes charge excitations as well, the condition manifests itself as the k dependence in the coupling constant.

Now the opposite limit of strong correlation is more interesting, since the weak-correlation picture should be drastically altered there. The most crucial question is

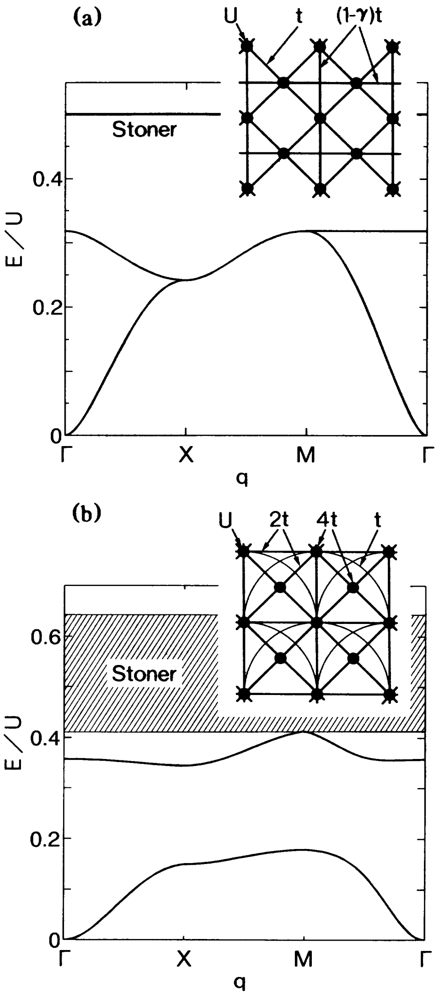

FIG. 1. Spin-wave modes (solid curves) and Stoner excitations in the weak-coupling regime in the 2D Mielke model with $\gamma = 0$ (a) and Tasaki's model (b) depicted in the insets. For the inset in (a) the flat band at the bottom of the single-electron dispersion for $\gamma = 0$ becomes dispersive for $\gamma \neq 0$.

whether the mass for the spin wave remains finite. Here we have to employ a completely different method, and we take a Roth type trial wave function [14,15] to represent the one-magnon state in the limit $U = \infty$. For multiband systems, we can write this function as

$$|\chi(\mathbf{q})\rangle \propto \sum_{\mathbf{k},\mathbf{r},m} e^{i(\mathbf{k}+\mathbf{q})\mathbf{r}} \psi_m(\mathbf{k}) C^\dagger_{\mathbf{r}+\mathbf{u}_m\downarrow}(1 - n_{\mathbf{r}+\mathbf{u}_m\uparrow}) C_{l\mathbf{k}\uparrow}|F\rangle, \quad (4)$$

where $\psi_m(\mathbf{k})$ is an amplitude which should be determined by solving a scattering problem, and the flat band is assumed to be the lowest branch in the single-electron dispersion as is the case with Mielke's and Tasaki's models. The summand represents that the annihilation of $\uparrow$ spin from the flat band is followed by a creation of $\downarrow$ spin at each *site* with the Gutzwiller projection, and this incorporates both the correlation effect and the interband effect, since the exclusion of doubly occupied sites involves multiband processes. $|\chi(\mathbf{q})\rangle$ includes both spin wave and Stoner (charge) excitations as does the weak-coupling expression. In the above trial function the Gutzwiller projection operates on the ferromagnetic Fermi sea, so that we implicitly assume that the contribution of the components in which the Fermi sea interior is disturbed is not appreciable for low-lying excitations.

We can now minimize the excitation energy, $\xi(\mathbf{q}) = \langle\chi(\mathbf{q})|H-E_0|\chi(\mathbf{q})\rangle$, for each value of $\mathbf{q}$, where E_0 is the energy of the ferromagnetic ground state. By varying ψ_m^*, we obtain a set of eigenvalue equations,

$$\sum_n K_{mn}(\mathbf{k};\mathbf{q})\psi_n(\mathbf{k}) + \frac{1}{N_a}\sum_{\mathbf{p}\neq\mathbf{k},n} L_{mn}(\mathbf{k},\mathbf{p};\mathbf{q})\psi_n(\mathbf{p}) = \xi(\mathbf{q})\left[(1-\langle n_m\rangle)\psi_m(\mathbf{k}) + \frac{1}{N_a}\sum_{\mathbf{p}\neq\mathbf{k}} \phi_{lm}^*(\mathbf{p})\phi_{lm}(\mathbf{k})\psi_m(\mathbf{p})\right]. \quad (5)$$

Here the kernels, K_{mn} and L_{mn}, are given in terms of a Fourier transform of $\phi_{\nu m}^*(\mathbf{k})\phi_{\nu n}(\mathbf{k})$, where the band index ν runs over l (flat band) and dispersive ones.

The eigenvalue equation above is applicable to any multiband model in which the bottom band (flat or dispersive) is filled by ↑ electrons. We have solved the equation numerically for finite systems with periodic boundaries, in which sample-size dependence turned out to be small.

Figure 2 shows the dispersion relation extrapolated to the infinite system by assuming that the size dependence disappears as $O(1/N_a)$. We immediately recognize the similarity with the weak-coupling result: the gapless Goldstone mode (acoustic magnon) along with the optical magnon modes (with a spatially oscillating spin-spin correlation) below the nearly flat charge (Stoner) gap. The essential difference is that both the spin-wave stiffness and Stoner gap are now of the order t rather than something like t^2/U = infinitesimal as one might naively expect. [Numerically, the charge gap is $E_G = 2.88t$ ($5.13t$) for Mielke's (Tasaki's) model, while the stiffness D in the spin-wave spectrum $\xi_{\mathrm{SW}}(\mathbf{q}) = Dq^2$ for small q is $D = 0.19t$ ($D = 0.37t$) for Mielke's (Tasaki's) model.]

The finite spin stiffness and a charge gap contrast with those in the more subtle Nagaoka ferromagnetism in the single-band Hubbard model. We can identify the difference by evoking the discussion of the latter by Shastry, Krishnamurthy, and Anderson [15]. The energy required to flip a spin, $\xi(\mathbf{q})$, is a sum of an energy to take out a ↑ electron, an energy to add a ↓ electron in the down spin band, and a positive scattering energy of the ↑ Fermi sea. The sum scales like the hole concentration from the half filling, $\delta = 1 - \langle n\rangle$. This reflects the reduced effective bandwidth of the down spin, which can only hop to vacant sites due to the strong correlation. For Nagaoka's case doped with a single hole (with $\delta = 1/N$ = infinitesimal), the mass of the spin-wave mode below the Stoner gap ($\xi \propto \delta$) becomes infinitely heavy ($\propto 1/\delta$). In the flat-band ferromagnetism, by contrast, the single-particle mass is infinitely heavy, but the electron correlation renders the spin-wave mass $\sim t$ even for $U = \infty$. This is because, although the flat band is half filled, higher bands are empty, leaving the occupation number per *site* less than unity. Further, the energy of the correlated down-spin electron is always elevated from the lowest single-particle state which is just the flat band itself. This means that the above sum is positive finite in the flat-band system, and we end up with a finite $\xi(\mathbf{q})$ with a singular dependence on δ absent.

The above results enable us to expect that ferromagnetism should survive when the flat band is made dispersive

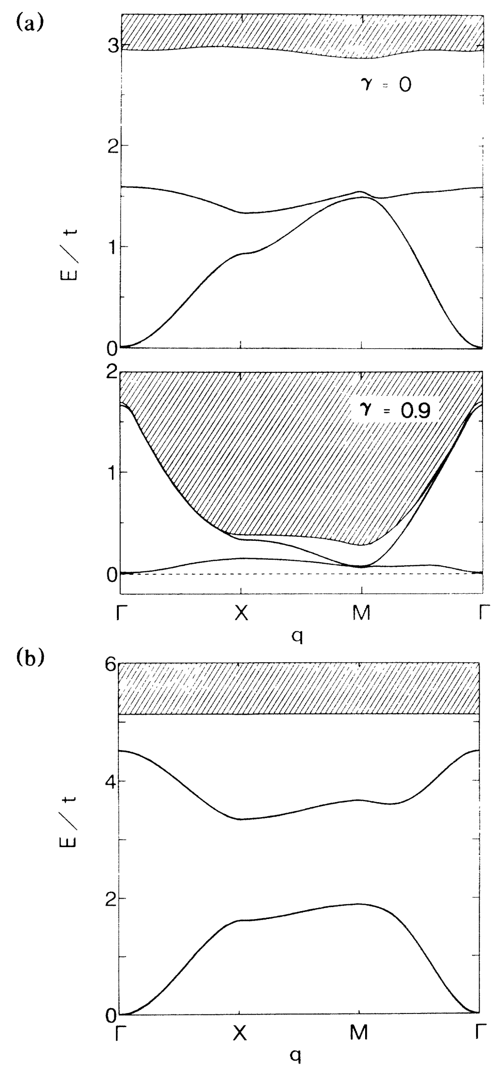

FIG. 2. (a) Spin-wave excitations (solid lines) and a scattering continuum (hatched regions) for Mielke's model with $\gamma = 0$ (upper panel) and for $\gamma = 0.9$ (lower panel) in the strong-coupling limit ($U = \infty$). (b) Spin-wave excitations (solid lines) and a charge excitation continuum (hatched region) for Tasaki's model

up to a finite extent. When we introduce a parameter γ in Mielke's model [Fig. 1(a)] to make the flat band dispersive, ferromagnetism should disappear at least in the small U limit. In the large U limit, however, a finite gap in the charge excitation implies that a finite γ should be required to destroy ferromagnetism. For $\gamma=1$, the half-filled flat band in Mielke's model becomes the quarter-filled, single-band square lattice, which is beyond the critical hole concentration, $\delta_c=0.49$, for the vanishing charge and spin-wave excitation energies at the Brillouin zone corner in the square lattice found by Shastry, Krishnamurthy, and Anderson [15]. Our calculation of the change in the energy spectrum against γ [Fig. 2(a)] using the function, Eq. (4), in the strong-coupling limit indeed shows that a dip in the charge gap and spin-wave dispersion appear at the M point (while the optical magnon mode is eventually absorbed in the Stoner continuum).

The acoustic spin wave softens at $\gamma_c=0.915$, but there is an indication that the actual breakdown of ferromagnetism occurs prior to this, accompanied by a discontinuous change in the total spin. A phase diagram on the (γ,U) plane obtained from a numerical diagonalization of finite systems [16] shows that the ferromagnetic phase exists for $U \geq U_c(\gamma)$, which diverges at $0.4<\gamma_c<0.5$. At the boundary a level crossing occurs between the fully spin-polarized state and a paramagnetic one (with $S \simeq 0$). The level crossing is also expected from the result of Putikka, Luchini, and Ogata [17] that the singlet ground state is lower in energy than the ferromagnetic state by a significant amount at $\gamma=1$. At any rate, the finite γ_c confirmed here again implies an itinerant ferromagnetism for finite bandwidths.

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