Spiral magnets as gapless Mott insulators

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Abstract

In the large $U$ limit, the ground state of the half-filled, nearest-neighbor Hubbard model on the triangular lattice is the three-sublattice antiferromagnet. In sharp contrast with the square-lattice case, where transverse spin-waves and charge excitations remain decoupled to all orders in $t/U$, it is shown that beyond leading order in $t/U$ the three Goldstone modes on the triangular lattice are a linear combination of spin and charge. This leads to non-vanishing conductivity at any finite frequency, even though the magnet remains insulating at zero frequency. More generally, non-collinear spin order should lead to such gapless insulating behavior.

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In band theory, insulating behavior is due to the existence of an energy gap in the single-particle excitation spectrum. It is well known, however, that interactions neglected in band theory may lead to insulating properties, a point first discussed by Mott and, in 1964, by Kohn who showed that the existence of an energy gap is sufficient but not necessary to have an insulator [1]. An insulator is thus best defined by a vanishing zero-temperature DC conductivity. In the usual examples of Mott insulators, however, there is generally a gap not only in the single-particle excitations, but also in the frequency dependent conductivity which is related to excited states at constant number of particles (particle-hole excited states instead of single-particle excitations). In this letter, we show that when interactions lead to
magnetic order in itinerant spin 1/2 systems, the resulting Mott insulator generally has no gap in the frequency dependent conductivity: This is the behavior of a gapless insulator. It is only when the magnetic order is collinear antiferromagnetism on hypercubic lattices that one can demonstrate the existence of a gap in the conductivity. In the general case that we consider in detail, the mixed spin and charge character [2] of the finite \( q \) collective (Goldstone) modes leads to the vanishing of the gap in the conductivity for a finite range of interaction strengths, despite the fact that the single-particle excitations do have a gap.

We start from the general one-band Hubbard model

\[
H = - \sum_{(i,j),\sigma} t_{ij} \left( c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma} \right) + U \sum_i n_{i\uparrow} n_{i\downarrow},
\]

where the first sum is over pairs of sites, \( t_{ij} \) is the hopping integral and \( U \) the on-site Coulomb interaction. We then define

\[
S^\mu(i) \equiv \frac{1}{2} \sum_{\alpha,\beta} c_{i\alpha} \sigma^\mu_{\alpha\beta} c_{i\beta},
\]

a dimensionless four-component spin and charge operator. (To be explicit, we let the matrix index \( \mu \) take the values \( \rho, x, y, z \), and we define \( \sigma^\rho \) as the unit matrix.) We consider the general class of magnetically ordered states with planar spiral order

\[
\langle S_z^\alpha \rangle + i \langle S_x^\alpha \rangle = S e^{iQ \cdot R_i},
\]

where \( S \) is the order parameter representing the average moment on each site. Without loss of generality, we take the spiral in the \( x - z \) plane. Well known examples of such states include the collinear antiferromagnet on the square lattice, \( Q = \pi/a \hat{x} + \pi/a \hat{z} \), and the three-sublattice antiferromagnet occurring on the frustrated triangular lattice, a 120\(^\circ\) spiral with \( Q = 4\pi/3a \hat{x} \). As always when working with planar spiral order, the analysis is greatly simplified by using a rotating (orthonormal) basis in which the quantization axis at every site points in the same direction as the average spin density of Eq.(3). In this rotating frame, the single-particle Green’s function

\[
\tilde{G}(i,j;i\omega_n) = T_i^\dagger G(i,j;i\omega_n) T_j,
\]

becomes, in matrix notation,
where the rotation matrix in spin space \( T_i = e^{-i(Q \cdot R_i) \sigma^y / 2} \) (with \( \sigma^y \) the usual Pauli matrix) depends on the site \( i \). In this reference frame, the Green’s function matrix \( \tilde{G} \) has the full underlying lattice periodicity, even for incommensurate spiral order. In the Hartree-Fock approximation, we find

\[
\tilde{G}(k, i\omega_n) = \frac{A_+(k)/2}{i\omega_n + \mu - E_+(k)} + \frac{A_-(k)/2}{i\omega_n + \mu - E_-(k)},
\]

(5)

where

\[
A_{\pm}(k) \equiv \begin{pmatrix} 1 & \Delta E_{\pm}(k) \\ \mp \frac{\eta_{\pm}(k)}{E(k)} & 1 \pm \frac{\Delta}{E(k)} \end{pmatrix}
\]

with the definitions

\[
\epsilon_0(k) \equiv -\frac{1}{N} \sum_{i,j} t_{ij} \cos k \cdot (R_i - R_j)
\]

for the single-particle dispersion in the paramagnetic phase (\( N \) is the number of sites), and

\[
\begin{align*}
\epsilon_\pm & \equiv \epsilon_0(k \pm Q/2) & \eta(k) & \equiv \frac{\epsilon_+(k) - \epsilon_-(k)}{2} \\
\epsilon(k) & \equiv \frac{\epsilon_+(k) + \epsilon_-(k)}{2} + \frac{U}{2} & \Delta & \equiv US \\
E(k) & \equiv \sqrt{\eta^2(k) + \Delta^2} & E_\pm(k) & \equiv \epsilon(k) \pm E(k)
\end{align*}
\]

(6)

The gap equation is given by the self-consistency requirement,

\[
\frac{U}{2N} \sum_k \left[ f(E_-(k)) - f(E_+(k)) \right] = 1,
\]

(7)

where \( f(x) \) is the Fermi function and the wave vector \( k \) spans the entire paramagnetic Brillouin zone of the crystal. The chemical potential is determined by number conservation,

\[
\frac{1}{N} \sum_k [f(E_-(k)) + f(E_+(k))] = 1.
\]

Proceeding to the collective excitations in the ordered state, we define the matrix response function

\[
\chi^{\mu\nu}(i, j; \tau) \equiv - \langle TS^\mu(i; \tau)S^\nu(j; 0) \rangle + \langle S^\mu(i) \rangle \langle S^\nu(j) \rangle.
\]

\( \chi \) is obtained in the Generalized Random-Phase Approximation (GRPA) by the usual summation of bubble and ladder diagrams. Since the GRPA is conservative, going beyond this
approximation should not change the qualitative aspects of ours results. In the rotating frame where $\chi^{\mu\nu}(i, j; \tau) \rightarrow \tilde{\chi}^{\mu\nu}(i - j; \tau)$, the matrix GRPA equation \[^3\] takes the form

$$\tilde{\chi}(\mathbf{q}, i\Omega_n) = \tilde{\chi}^0(\mathbf{q}, i\Omega_n) + 2U\tilde{\chi}^0(\mathbf{q}, i\Omega_n)\Gamma\tilde{\chi}(\mathbf{q}, i\Omega_n),$$

(8)

where $\Gamma$ is a diagonal matrix with $\Gamma^{\rho\rho} \equiv 1$, $\Gamma^{xx} \equiv \Gamma^{yy} \equiv \Gamma^{zz} \equiv -1$.

At $T = 0K$, which we will consider from now on, the retarded zeroth-order matrix susceptibility $\tilde{\chi}^0(\mathbf{q}, \omega + i\delta)$ is given by,

$$\tilde{\chi}^0(\mathbf{q}, \omega + i\delta) = \frac{1}{8N} \sum_k \left( \begin{array}{cccc}
-\Delta_+ & \frac{n-n'}{E'E''} & \frac{n-n'}{E'E''} & -\Delta_+ \\
-\Delta_- & \frac{n-n'}{E'E''} & \frac{n-n'}{E'E''} & -\Delta_- \\
\frac{n-n'}{E'E''} & \Delta_+ & \frac{n-n'}{E'E''} & \Delta_- \\
\frac{n-n'}{E'E''} & \Delta_- & \frac{n-n'}{E'E''} & \Delta_+
\end{array} \right)
$$

(9)

where unprimed functions are to be evaluated at $\mathbf{k}+\mathbf{q}/2$ and the primed functions at $\mathbf{k}-\mathbf{q}/2$, and where $\Lambda_\pm \equiv \gamma_- \pm \gamma_+$ with

$$\gamma_\pm = \frac{1}{\omega + i\delta - (E - E')} \pm (E + E').$$

(10)

The response function in the rotating frame $\tilde{\chi}$ can be related to the laboratory response $\chi$ but the expressions are lengthy \[^3\]. For the density response however, the relation simply is

$$\chi^{\rho\rho}(\mathbf{q}, \mathbf{q}', \omega + i\delta) = \tilde{\chi}^{\rho\rho}(\mathbf{q}, \omega + i\delta)\delta_{\mathbf{q}, \mathbf{q}'}.$$  

(11)

The other response functions involve linear combinations of $\tilde{\chi}$ at different wave-vectors. The poles of $\tilde{\chi}$, which of course coincide with those of $\chi$, give the position of the collective modes.

For hypercubic lattices in arbitrary dimension larger than one, symmetry arguments can be used to show that whatever the hopping matrix $t_{ij}$ and the value of $U$, as long as there is long-range collinear antiferromagnetic order, the response matrix $\tilde{\chi}$ is block diagonal. There are then two Goldstone modes with purely transverse $x - y$ character. For the nearest-neighbor model at half-filling, it is well known \[^4\] that in the limit $t \ll U$, the above
approach correctly reproduces the standard spin wave result of the Heisenberg model with 
\[ J \sim 4t^2/U. \] For next-nearest neighbor hopping on the square lattice, the resulting spin Hamiltonian in the large \( U \) limit is frustrated. Nevertheless, it follows from above that as long as there is long-range antiferromagnetic order, there are two Goldstone modes with purely transverse \( x - y \) character, as in the simpler non-frustrated case.

From now on, we restrict ourselves to the nearest-neighbor triangular lattice at half-filling. On this lattice, the frustrated antiferromagnetism can give rise to non-collinear magnetic order, a subject of current interest in itself \[5\]. Much work has been done to obtain the magnetic phase diagram as the electrons are allowed to be more and more itinerant (\textit{i.e.} as the ratio \( U/t \) decreases) \[6\]. Krishnamurthy \textit{et al.} \[7\] and Jayaprakash \textit{et al.} \[8\] have shown that, at half-filling, as \( U \) is increased the Hartree-Fock ground-state evolves from a paramagnetic metal to a metallic incommensurate spiral Spin-Density-Wave (SDW) then to a commensurate linear SDW with indirect gap and finally, at higher values of \( U \), into a spiral SDW insulator with a three-sublattice 120° twist between spins on neighboring sites. This spiral (or equivalently helical) SDW state is the well known ground state of the Heisenberg model (with \( J \sim 4t^2/U \)). We call this state the 120° spiral SDW phase.

We go beyond previous studies by accounting for the collective excitations of the 120° spiral SDW phase. The electronic dispersion in the absence of interaction for the nearest-neighbor model on the triangular lattice is given \[9\] by 
\[ \epsilon_0(k) = -2t(\cos(k_xa) + 2\cos(k_xa/2)\cos(\sqrt{3}k_ya/2)). \]
In the paramagnetic Brillouin zone, the single band \( \epsilon_0(k) \) is split into the two subbands \( E_{\pm}(k) \) by the presence of spiral order, as can be seen from Eqs.(5),(6). The direct single-particle energy gap is \( 2\Delta \) but the indirect gap \( E_{IG} = \text{Min}[E_+(k)] - \text{Max}[E_-(k)] \) can be lower than this value. When the indirect gap vanishes, a transition to a metallic state occurs. This transition takes place at a value of \( t/U \approx 0.195 \), above which the order parameter \( S \) decreases very rapidly. However, the collective modes destabilize the insulating 120° spiral SDW phase at \( t/U \approx 0.146 \), well before the above metallic transition is reached. In the following, we restrict ourselves to the regime at half-filling where the indirect gap is positive and only the lowest energy band is filled.
Expanding $\tilde{\chi}^0(q, \omega)$ Eq.(4) to second order in $\omega/U, t/U$, and using the gap equation to eliminate $S$ in favor of $U$, we find after tedious algebra that to leading order in $t/U$, the poles $\omega(q)$ of the response function Eq.(8) correctly reproduce the standard spin wave result of the Heisenberg model with $J = 4t^2/U$ [10]. If $q$ is restricted to the magnetic Brillouin zone, the three spin-wave branches (Goldstone modes) are given by $\omega(q), \omega(q + Q), \omega(q - Q)$.

As the ratio $t/U$ increases and the electrons become more itinerant, higher-order terms in $t/U$ cannot be neglected and the coupling between charge and the three spin components becomes important. The matrix $\tilde{\chi}(q, \omega)$ is no-longer block diagonal and all response functions then share the same poles, although with different weights. Three of the poles are still Goldstone modes with a vanishing frequency at $q = 0$ in the magnetic Brillouin zone. In Fig. 1 we plot the imaginary part of the response functions $\tilde{\chi}^{\rho\rho}$ and $\tilde{\chi}^{xx}$ for various values of $q$. We plot in Fig.2 the dispersion relation of the collective modes obtained by following the peak of the response function as $q$ is varied along high-symmetry directions.

It is clear from Fig. 1 that the coupling between spin and charge is very small so that the spin waves are only very slightly modified by the charge fluctuations. The intensity of this coupling increases with $t/U$ but there is only a narrow range of $t/U$ over which the $120^0$ spiral SDW is stable. Indeed, at $t/U \approx 0.146$ one of the collective modes softens, destabilizing the $120^0$ spiral SDW ground state at a smaller value than the $t/U = 0.16$ found in Ref. [8] using only self-consistent Hartree-Fock solutions.

Because the collective modes with coupled spin-wave and charge extend to zero-frequency, it is natural to ask whether the system could becomes conducting despite the existence of a gap in the single-particle excitations. The appropriate definition of an insulator is that it has a vanishing Drude weight. [1,11] This statement is equivalent to saying that the coefficient of the delta function $\delta(\omega)$ in the zero-temperature DC conductivity $\sigma_{DC} = \lim_{\omega \to 0} \lim_{q \to 0} \sigma(\omega, q)$ vanishes. We obtained this quantity from the appropriate limit of

$$\sigma(\omega, q) = ie^2 \frac{\omega + i\delta}{q^2} \chi^{\rho\rho}(\omega + i\delta, q, q).$$

(12)

In this expression, one has to take the part of $\chi^{\rho\rho}(\omega + i\delta, q, q) = \tilde{\chi}^{\rho\rho}(\omega + i\delta, q, q)$ which is
irreducible with respect to the interaction. \[12\] This eliminates the effect of screening. Expanding to second order in \(q, \omega\), we found after lengthy algebra that the charge-response function decreases faster than \(q^2\) for \(q \to 0\) so that the Goldstone-mode contributing to \(\sigma(\omega, q)\) has effectively zero weight at \(q \to 0\). The same conclusion is reached by calculating the transverse current-current response function in the GRPA. It then follows that the system remains insulating even though there is no gap in the charged collective excitations. This is not so surprising since at \(q = 0\) the Goldstone modes restore rotational invariance: hence they have the same parity as the ground state so that matrix elements of the current operator between the \(q = 0\) modes and the ground state vanish.

At finite wave vector and frequency, however, the conductivity is finite and, as shown in Fig. 3, the absorption described by the real part is exactly at the Goldstone-mode position, as expected. We conjecture that the insulator can be changed into a bad conductor by impurities. Indeed, impurities transform the single delta function \(\delta(\omega)\) appearing in the \(DC\) conductivity of perfect metals into a Lorentzian-like response. In our case, the breaking of crystal momentum conservation by impurities would probably, by a similar mechanism, broaden the finite \(q\) resonances to make the \(q = 0\) conductivity finite everywhere in the single-particle gap, including zero frequency. The question is difficult because of possible Anderson localization.

In conclusion, the triangular three-sublattice antiferromagnet described by the large \(U\) half-filled one-band Hubbard model provides an example of a gapless Mott insulator. In this system, the Goldstone modes have mixed spin and charge character, leading to the disappearance of the gap in the conductivity, despite a vanishing \(DC\) conductivity and the existence of a gap in the single-particle excitations. This phenomenon is generic for itinerant magnets with spiral order. An exception is when the ordering wave vector corresponds to collinear antiferromagnets.

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FIGURES

FIG. 1. Imaginary part of the density and (inset) spin response functions at $t/U = 0.1$. From left to right the peaks, broadened by a small imaginary part, correspond to $q_y = 0, q_x = 0.1, 0.15, 0.25$ (in units of $2\pi/a$)

FIG. 2. Dispersion relation of the mixed spin and charge collective modes along the edges of the irreducible Brillouin zone of the triangular lattice. The full, dashed and dot-dashed curves are respectively for $t/U = 0.1, 0.12, 0.146$.

FIG. 3. Real part of the conductivity defined in Eq. (13) at $t/U = 0.1$ and for the wave vectors $q_y = 0; q_x = 0.1, 0.15, 0.25$ (in units of $2\pi/a$) represented by the full, dashed and dot-dashed curves respectively.
-Im [U χ ρ ρ]

[Diagram of a graph showing peaks at ω/U = 0.02 and 0.04]
