Excitations near the boundary between a metal and a Mott insulator

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Abstract. A heterostructure of a semi-infinite metal and a Mott insulator is considered. It is supposed that both materials have an identical lattice spacing and hopping integrals and differ in the Hubbard repulsion which is negligible in the metal and exceeds the critical value for the Mott transition in the insulator. At half-filling and for low temperatures the insulator has long-range antiferromagnetic order. Its low-lying elementary excitations are standing spin waves and a spin-wave mode which is localized near the interface and has a two-dimensional dispersion. This mode ejects bulk modes from the boundary region. The antiferromagnetic ordering of the insulator induces an antiferromagnetic order in the metal where the magnetization decays exponentially with distance from the interface. This decay is characterized by the correlation length of about 6 lattice spacings.

In the last few years an active interest has been taken in heterostructures fabricated out of crystals with strong electron correlations. Looking for new effects and their possible applications a wide variety of systems has been investigated both experimentally and theoretically (see, e.g., [1]). In this paper, we study a heterostructure of this type which consists of a metal and a Mott insulator. The two crystals are supposed to have the same simple cubic lattice structure with identical hopping constants and differ only in the value of the Hubbard on-site repulsion U which vanishes in the metal and exceeds the critical value for the Mott transition $U_c \approx 2.8B$ [2] in the insulator. Here $B = 6|t|$ is the electron band halfwidth and $t$ is the hopping integral between nearest neighbor sites. At half-filling the penetration of the metallic state into the Mott insulator is negligibly small [2] and the spin excitations are its only low-lying excitations.

The small ratio $|t|/U$ allows us to simplify the problem by applying a unitary transformation which is similar to that used for the derivation of the $t$-$J$ Hamiltonian from the Hubbard Hamiltonian [3]. The transformed Hamiltonian reads

$$H = t \sum_{l \sigma} \sum_{t_x \leq -1} a^\dagger_{l+a,l_x \sigma} a_{l_x \sigma} + t \sum_{l \sigma} \sum_{t_x \leq -1} \left( a^\dagger_{l+l_x-1,\sigma} a_{l_x \sigma} + a^\dagger_{l+l_x \sigma} a_{l_x-1,\sigma} \right) + J \sum_{l \sigma} \sum_{t_x \geq 0} S_{l+l_x} S_{U_x} + J \sum_{l \sigma} \sum_{t_x \geq 0} S_{l+l_x+1} S_{U_x} + 2J \sum_{l \sigma} \left( S_{U_x} S_{l+1} - \frac{1}{4} \sum_{\sigma} X^\sigma_{l+1} \right), \quad (1)$$

where $t_x$ and $l = (l_y, l_z)$ label sites of the lattice, $a$ are 4 vectors connecting nearest neighbor sites in the yz plane, $a_{l_x \sigma}$ is the electron annihilation operator with the spin projection $\sigma$, $J = 4t^2/U$ is the exchange constant, $S_{U_x}$ is the spin-$\frac{1}{2}$ vector and $X^\sigma_{l_x} = |U_x \sigma\rangle\langle U_x \sigma|$ is the
Hubbard operator with the singly occupied site state $|l_x, \sigma\rangle$. The metal is located in the half-space $l_x \leq -1$, while the insulator is in the half-space $l_x \geq 0$. The lattice spacing is taken as the unit of length. Notice that the exchange constant between the boundary layers $l_x = -1$ and $l_x = 0$ is twice as large as the constant in the Mott region.

Equation (1) contains Hamiltonians of the semi-infinite metal (the first and second terms on the right-hand side of this equation) and of the semi-infinite antiferromagnet (the third and fourth terms). The former Hamiltonian is brought to the diagonal form in terms of the operators and eigenenergies

$$a_{kk', \sigma} = \sqrt{\frac{2}{\pi N}} \sum_1 e^{-ikl \sin(k_x l_x) a_{l_x, \sigma}}, \quad \varepsilon_{kk'} = 6t \gamma_{kk'}^{(3)},$$

where $\gamma_{kk'}^{(3)} = \frac{1}{3} [\cos(k_z) + \cos(k_y) + \cos(k_x)]$, $N$ is the number of sites in the periodic $yz$ plane, $k = (k_y, k_z)$, $-\pi < k_y, k_z \leq \pi$ and $0 < k_x < \pi$. Operator (2) corresponds to a running wave for the directions $y$ and $z$ and to a standing wave for the direction $x$.

The situation is more complicated for the antiferromagnet. Using the spin-wave approximation [4] we define the two-component operator $\hat{B}_{kl} = (b_{kl}^x, b_{-kl}^z)$ and the matrix retarded Green’s function

$$\hat{D}(ktl_x t_x') = -i\theta(t) \langle \{\hat{B}_{kl}^x (t), \hat{B}_{kl}^z (-t, l_x)\} \rangle ,$$

where the averaging and the time dependence are determined with the Hamiltonian of the antiferromagnet, $b_{kl}^x$ and $b_{kl}^z$ are the spin-wave operators which satisfy the boson commutation relations. The equation of motion for Green’s function (3) reads

$$\frac{i}{2} \frac{d}{dt} \hat{D}(ktl_x t_x') = \delta(t) \delta_{l_x} \Theta_x + J \left[ 3\left(1 - \frac{1}{6} \delta_{l_x} \right) \hat{\tau}_z + 2i \gamma_k^{(2)} \hat{\tau}_y \right] \hat{D}(ktl_x t_x')$$

$$+ i \frac{J}{2} \hat{\tau}_y \left[ \hat{D}(kt, l_x - 1, t_x') + \hat{D}(kt, l_x + 1, t_x') \right] ,$$

where $\hat{\tau}_y$ and $\hat{\tau}_z$ are Pauli matrices and $\gamma_k^{(2)} = \frac{1}{7} [\cos(k_y) + \cos(k_z)]$. If we define $\hat{D}^{(0)}(ktl_x t_x')$ as Green’s function which satisfies Eq. (4) without the term proportional to $\delta_{l_x} \Theta_x$ and associated with broken bonds on the surface, the solution of Eq. (4) can be written as

$$\hat{D}(ktl_x t_x') = \hat{D}^{(0)}(ktl_x t_x') - \frac{J}{2} \int_{-\infty}^{\infty} dt' \hat{D}^{(0)}(k, t' - t, l_x 0) \hat{D}(kt' 0 l_x').$$

After the Fourier transformation we find finally

$$\hat{D}(k\omega l_x t_x') = \hat{D}^{(0)}(k\omega l_x t_x') - \frac{J}{2} \hat{D}^{(0)}(k\omega l_x 0) \left[ \hat{I} + \frac{J}{2} \hat{D}^{(0)}(k\omega 0) \right]^{-1} \hat{D}^{(0)}(k\omega 0 l_x'),$$

where $\hat{I}$ is the $2 \times 2$ unit matrix.

Green’s function $\hat{D}^{(0)}(k\omega l_x t_x')$ can be calculated using the Bogoliubov-Tyablikov transformation for the diagonalization of quadratic forms [4]. Elementary excitations described by this function are standing spin waves with the dispersion

$$E_{kk'} = 3J \sqrt{1 - \left(\frac{\gamma_{kk'}^{(3)}}{\gamma_{kk'}^{(3)}\gamma_{kk''}^{(3)}}\right)^2} .$$

The spectral functions corresponding to Green’s functions $\hat{D}(k\omega l_x t_x')$ and $\hat{D}^{(0)}(k\omega l_x t_x')$ are shown in Fig. 1. On the surface, $l_x = 0$, the peak arising from the pole of the second term on the right-
hand side of Eq. (5) dominates in the spectrum (see Fig. 1a). However, already at $l_x = 5$ the peak disappears in the continuum of standing waves – the spectra $\text{Im}D_{11}(k\omega l_x l_x)$ and $\text{Im}D_{11}^{(0)}(k\omega l_x l_x)$ are practically identical in Fig. 1b. Thus, the peak corresponds to a surface spin-wave mode. Its dispersion can be derived from $\text{Im}D_{11}(k\omega l_x l_x)$ for $l_x = 0$,

$$\omega_k = 2J' \sqrt{1 - \left(\frac{\gamma(2)}{\gamma_k}\right)^2},$$

where $J' \approx 1.23J$. It is the dispersion of 2D spin waves with a somewhat enlarged exchange constant. Notice that the surface mode ejects the bulk modes, i.e. the standing waves, from a few surface layers. In Fig. 1a the latter modes are seen as a weak shoulder on the high-frequency side of the surface peak. The situation is similar to the impurity problem where localized states extrude bulk modes from the defect region [5].

In the zeroth order values of the spin operators $S_{l-1}$ in the last (interaction) term of Hamiltonian (1) are zero. Therefore spin excitations of the Mott part of the heterostructure are close to those which were considered above.

Now we consider the influence of the long-range antiferromagnetic ordering of the Mott insulator on the magnetic state of the metal. In accord with the idea of the spin-wave approximation which considers spin-wave excitations as small deviations from an equilibrium state, the Hamiltonian can be written as

$$H = H_0 + H_I,$$

where $H_0$ is the Hamiltonian of the Mott insulator and $H_I$ is the interaction term.

Figure 1. The imaginary parts of Green’s functions $D_{11}(k\omega l_x l_x)$ (solid lines) and $D_{11}^{(0)}(k\omega l_x l_x)$ (dashed lines) for $l_x = 0$ (a) and $l_x = 5$ (b). $k = (0, 0.6\pi)$. In part (a), the dash-dotted line displays the real part of the denominator in the second term on the right-hand side of Eq. (5).

Figure 2. (a) The magnetization $M$ in the metal as a function of the distance from the surface $l_x$ for $J = 0.23|t|$ and the temperature $T = 0$. (b) The absolute value of $M$ in a semi-logarithmic scale for $T = 0$, $J = 0.23|t|$ (filled circles) and $J = 0.1|t|$ (open circles).
orientation, we keep only the largest interaction term in Hamiltonian (1) which reads

$$\hat{J} \frac{1}{2} \sum_{\mathbf{q} \sigma} e^{i \mathbf{Q} \cdot \mathbf{a}_{\mathbf{q} \sigma}} a^{\dagger}_{\mathbf{q} \sigma} a_{\mathbf{q} \sigma},$$  

(8)

where $\mathbf{Q} = (\pi, \pi)$. We are interested in the magnetization $M_{\mathbf{q}} = n_{\mathbf{q} \uparrow} - n_{\mathbf{q} \downarrow}$ in the metal region. Here $n_{\mathbf{q} \sigma} = a_{\mathbf{q} \sigma}^{\dagger} a_{\mathbf{q} \sigma}$. This quantity can be obtained from Green's function

$$G_{mn}(\mathbf{q} l z l') = -i \theta(t) \left\langle \left\{ a_{\mathbf{q} m l z \sigma}(t), a^{\dagger}_{\mathbf{q} m l' z' \sigma} \right\} \right\rangle$$  

(9)

with the operators $a_{\mathbf{q} m l z \sigma}, m = 1, 2$, determined in the magnetic Brillouin zone. Since the term (8) divides the yz plane into two sublattices, it is convenient to use this zone which is half as much as the usual 2D Brillouin zone. The index $m$ is introduced to allow for the smaller number of wave vectors $\mathbf{q}$ in the former zone. The equation for this Green’s function can be obtained in the same manner as above for $D(\mathbf{k} \omega l x l')$,

$$\hat{G}(\mathbf{q} l x l', \sigma) = \hat{G}^{(0)}(\mathbf{q} l x l', -1) - \frac{J}{2} \sigma \hat{G}^{(0)}(\mathbf{q} l x l', -1) \tau_z \left[ \hat{I} + \frac{J}{2} \sigma \hat{G}^{(0)}(\mathbf{q} \omega, -1, -1) \tau_z \right]^{-1} \hat{G}^{(0)}(\mathbf{q} \omega, -1, l_x),$$  

(10)

where $\hat{G}^{(0)}(\mathbf{q} \omega l x l')$ describes the standing waves (2).

Results are shown in Fig. 2. The spins of electrons in the metal region are antiferromagnetically ordered (see Fig. 2a). The magnetization decays exponentially with distance from the boundary with the correlation length $\xi \approx 6$ lattice spacings. The correlation length depends only weakly on the ratio $J/|\mathbf{t}|$ in the considered range of this parameter (see Fig. 2b). The comparatively large value of $\xi$ yields the penetration of the antiferromagnetic order into the metal for distances of tens of lattice spacings. We considered the influence of other interaction terms of Hamiltonian (1) on this ordering and found that their contribution is small in comparison with the term (8). The ordering can be also interpreted as Friedel oscillations due to the effective magnetic field imposed by the antiferromagnetic order in the insulating side. Notice that in the case of Eq. (10) localized states do not arise, since in the denominator of the second term on the right-hand side $J$ is much smaller than the effective energy parameter of Green’s function $\hat{G}^{(0)}(\mathbf{q} \omega, -1, -1)$, i.e. the electron bandwidth in the metal.

In summary, the heterostructure of the semi-infinite metal and the Mott insulator was considered in the case of half-filling. It was found that for low temperatures the low-lying excitations of the insulator are standing spin waves and a surface spin-wave mode with 2D dispersion. This surface mode ejects the bulk spin waves from a few layers near the surface. The antiferromagnetic ordering of the insulator induces antiferromagnetic order in the metal with the magnetization decaying exponentially with distance from the boundary. The correlation length of this decay is about 6 lattice spacings.

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