Antiferromagnetism of the Hubbard Model on a Layered Honeycomb Lattice
– Is MgB$_2$ a Nearly-Antiferromagnetic Metal? –

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As a model for the B 2$p_z$ bands of MgB$_2$, a half-filled Hubbard model on a honeycomb lattice is studied, and a possibility of an antiferromagnetism (AF) at the ground state is examined by Monte Carlo calculations as well as a random phase approximation method. On a single-layer honeycomb lattice, a paramagnetic to AF phase transition occurs at a finite value of the repulsion energy $U_c/t \simeq 3.6$, due to the loss of the density of states at the fermi level. On a layered honeycomb lattice, however, inter-layer hopping term creates a perfect nesting of the fermi surface, and leads the AF with $U_c = 0$. From these facts, we discuss that MgB$_2$ is possibly a nearly-AF metal, where the AF of the 2$p_z$ bands is destroyed by carrier doping.

KEYWORDS: Hubbard model, honeycomb lattice, MgB$_2$, superconductivity, antiferromagnetism, nesting

§1. Introduction

The recent discovery of MgB$_2$, an intermetallic superconductor with high superconducting transition temperature ($T_c$), initiated a large number of activities both in experimental and theoretical researches. Several experiments, including NMR, specific heat, as well as photoemission spectrum measurements suggest that this material shows BCS-like $s$-wave superconductivity. Band calculations indicate a strong interaction between electrons and high-frequency phonon modes exists, which has been discussed as a possible origin of high $T_c$ superconductivity in this material. It has been also argued that roles of strong Coulomb interactions may directly or indirectly give rise to high $T_c$ superconductivity.

The crystal of MgB$_2$ consists of alternative stackings of honeycomb-lattice B$_2$ layers and triangular-lattice Mg layers, as is in AlB$_2$. The band calculations show that Mg are almost fully ionized, and the bands at the fermi level have mostly B 2$p_z$ characters. There exist four fermi surfaces, two of them in the 2$p_z$ bands and the rest in the 2$p_{x,y}$ bands. The 2$p_{x,y}$ bands are derived from the intra-layer $\sigma$ bonding orbitals, and have a quasi two-dimensional hole character. The 2$p_z$ bands are derived from the intra-layer $\pi$ bonding orbitals which also have inter-layer couplings between adjacent atomic orbitals in the $c$-axis direction.

The tight-binding fits to the band structure calculations show that the 2$p_z$ bands are well reproduced by a nearest neighbor (N.N.) hopping model on a layered honeycomb lattice of B sites in the formulae

$$\varepsilon_{\pm}(k) = \pm 2t_{xy}\gamma_{xy}(k) - 2t_z \cos(k_z),$$

$$\gamma_{xy}(k) = \sqrt{\frac{3}{4} + \frac{1}{2} \cos(k_x) + \cos\left(\frac{1}{2}k_x\right) \cos\left(\frac{\sqrt{3}}{2}k_y\right)},$$

where $t_{xy}$ ($t_z$) denotes intra-layer (inter-layer) N.N. electron hopping energy, while $\gamma_{xy}$ is the structure factor of the intra-layer electron hopping to the N.N. sites on a honeycomb lattice. A lattice structure of the tight-binding model is illustrated in Fig. 1.

![Fig. 1. Boron sites in the layered honeycomb lattice structure of MgB$_2$. Tight-binding fits show that a N.N. hopping model between boron sites reproduces the 2$p_z$ bands. Characters A and B denote sublattice indices.](image)

In this Letter, we investigate an aspect of the 2$p_z$ bands in MgB$_2$ which comes from its characteristic band
structure. We consider a Hubbard model on a layered honeycomb lattice. Using a random phase approximation (RPA) as well as quantum Monte Carlo (MC) methods, antiferromagnetism (AF) at the ground state is examined. We discuss that inter-layer electron hoppings create a perfect fermi-surface nesting in the 2$p_z$ bands. With infinitesimal values of the Coulomb repulsion, the system is unstable against an AF order at half filling.

First, let us consider a half-filled Hubbard model on a general bipartite lattice with N.N. hoppings. This model has a particle-hole symmetry, and as a result, a non-interacting electron dispersion has a relation

$$\epsilon(k + Q) = -\epsilon(k),$$

where $Q$ is the AF wavevector defined by the bipartite structure of the lattice, e.g. $Q = (\pi, \pi)$ for a square lattice. To be more precise, the relation (3) holds when an electron on a A-sublattice site hops only to sites on B-sublattice, and vice versa. A particle-hole symmetry gives the chemical potential

$$\mu$$

on a B-sublattice, and vice versa. A particle-hole symmetry

$$\text{stability occurs at a non-zero value of } U_0 = 1/\chi_0(Q).$$

The detailed calculation gives $U_0/t = 2.23$. In other words, the critical value for the SDW occurs at infinitesimal values of $\tau$. Here, $\mathcal{H}$ is the Hamiltonian of the Hubbard model with electron hopping energy $t$ and a repulsive interaction $U$. For the initial state $|\Psi_{\text{ini}}\rangle$, we use a Hartree-Fock solution for the identical lattice with an interaction $U_{\text{ini}}$. Note that $U_{\text{ini}} (\neq U)$ can be chosen arbitrarily, and an appropriate value for $U_{\text{ini}}$ accelerates the convergence to the ground state.

Monte Carlo runs are performed for various system sizes with linear dimension $L = 6, 8, 10, 12, 14$ and 16. We typically run 10,000 Monte Carlo steps after 1000 relaxation steps. AF structure factor is calculated by

$$S(Q) = \frac{1}{N} \sum_{i,j} S_i \cdot S_j (-1)^{r_i - r_j}. \quad (6)$$

Here $N$ is the number of sites. Staggered magnetization $M_s$ is obtained by

$$M_s^2 = \lim_{N \to \infty} S(Q)/N. \quad (7)$$

Therefore, existence of the AF order can be judged by the extrapolation of $S(Q)/N$ to the thermodynamic limit.

System size dependence of $S(Q)/N$ for various values of $U$ is depicted in Fig. 2. We extrapolate the data by $1/L$. Here, finite size effects due to linear spin-wave type excitations in the AF ordered states are assumed. From the data we see that the extrapolation gives $M_s > 0$ at $U/t \geq 3.7$. Meanwhile, at $U/t \leq 3.5$ the $1/L$ extrapolation gives negative values for $M_s^2$, indicating that $1/L$ dependence derived from the linear spin wave theory does not hold in this case. From this fact, the critical value for the onset of AF order is estimated to be $U_c/t \approx 3.6$. Thus, quantum fluctuations do not extinguish RPA instability. They only renormalize the value of $U_c/t$ by a factor of about 1.6. As long as the existence of the instability is concerned, RPA is considered to be reliable.

Next, we introduce inter-layer hoppings. For a while, we assume a half-filled situation for the $2p_z$ bands, of
which energy is described by eq. (1). In actual MgB$_2$, however, existence of hole fermi surfaces in the 2$p_{x,y}$ bands leads a deviation from half-filling for the 2$p_z$ bands. The doping effect will be discussed later.

As illustrated in Fig. 1, the lattice structure is bipartite. We take intra-layer and inter-layer N.N. hoppings only. An inter-sublattice hopping on a bipartite lattice creates a particle-hole symmetry. Indeed, a non-interacting electron dispersion in eq. (1) shows

$$\varepsilon_+ (k_x, k_y, k_z) = -\varepsilon_- (k_x, k_y, k_z + \pi).$$

(8)

Note that, since a unit cell contains two boron atoms and the first Brillouin zone is already halved by the crystallographic reason, the AF wavevector in this lattice is $Q = (0,0,\pi)$. As an inter-layer hopping $t_z$ is increased from zero, the energy dispersion along the $k_z$ axis makes the fermi surface expand from the lines in the Brillouin zone connecting K and H points, and creates fermi surfaces with finite surface volumes around $k_z = 0$ and $k_z = \pi$. Therefore, at $t_z \neq 0$, the DOS at the fermi level becomes non-zero. Then, from eq. (4), $\chi_0(Q)$ diverges logarithmically, and the RPA instability occurs at infinitesimal values of $U$.

This behavior can be understood as a creation of a fermi surface nesting by increasing the inter-layer electron hoppings. For any $k$-points on the fermi surface, the relation $\varepsilon_+ (k_x, k_y, k_z) = -\varepsilon_- (k_x, k_y, k_z + \pi) = 0$ holds, which means the perfect interband nesting with $Q = (0,0,\pi)$. The situation is schematically illustrated in Fig. 3. Increase of $t_z$ makes the surface volumes of the perfectly-nested fermi surfaces increases.

Enhancement of the nesting behavior by the inter-layer hoppings is in a great contrast with usual quasi low-dimensional systems where three dimensionality induces curvatures of the fermi surface and hence decreases nesting properties. This unique feature comes from the bipartite geometry of a honeycomb lattice.

Within this band structure, $U_c \neq 0$ holds strictly only at $t_z = 0$, while we suddenly have $U_c = 0$ at $t_z \neq 0$. $U_c$ behaves singularly as a function of $t_z$. In other words, for a small value of $U$, SDW order appears as soon as inter-layer hopping is allowed. In practice, however, there exist particle-hole symmetry breaking terms, e.g. second neighbor hoppings as well as a chemical potential shift due to carrier doping. Then, there exists a competition between the inter-layer hopping term which create the fermi surface nesting and the symmetry breaking terms which destroys the nesting. As a result, the singular behavior in the $t_z$ dependence of $U_c$ will be smeared out by the particle-hole symmetry breaking terms, and $U_c$ is speculated to remain non-zero. Nevertheless, as long as the particle-hole symmetry breaking terms are small, we expect that AF instability occurs at relatively small values of $U$.

If the 2$p_z$ bands of MgB$_2$ are half filled, the strong nesting behavior of the fermi surfaces creates an AF-SDW state even if the Coulomb repulsion is not so large. Therefore, it is possible that MgB$_2$ is a nearly-AF metal. Self-doped carriers from the 2$p_{x,y}$ bands to the 2$p_z$ bands might have destroyed the AF order and make MgB$_2$ nonmagnetic, being similar with the case for high-$T_c$ cuprates in the doped region. At this point, however, it is not clear whether such AF is correlated to the mechanism of the superconductivity in MgB$_2$, e.g. whether...
remnant AF fluctuations assist the phonon mechanism to enhance the attractive interaction for the Cooper pairing. Further detailed studies are required to address this question.

In this sense, lattice structure of MgB$_2$ is special because the layer stacking conserves the bipartite nature. As a counter example, we make a comparison with graphite, where stacking of the honeycomb layers are not similar to those for MgB$_2$. A carbon atom on an adjacent layer lies on top of the center of a hexagon, which is not a bipartite structure. Then, the system is stable against AF instabilities in the small $U$ region. This explains the fact that graphite does not show AF. Coulomb interactions are expected to be not strong enough to induce a magnetically ordered state.

In order to justify the idea that MgB$_2$ is a nearly-AF metal, we propose some crucial tests. From the band calculation, more precise estimate for the band dispersion, either by the tight-binding fits, or by directly calculating the fermi surface, will give how strong the nesting behavior is in this material. Coulomb repulsion energy should also be estimated to clarify whether it is strong enough to cause AF states if the 2$p_z$ bands are half filled. Experimentally, measurement of remnant AF spin fluctuations in MgB$_2$ is important. A search for AF states in various diboride compounds with half-filled 2$p_z$ bands is also interesting.

To summarize, ground state magnetism of the Hubbard model on a layered honeycomb lattice at half-filling is studied as a model for the B 2$p_z$ bands of MgB$_2$. RPA as well as MC calculations are performed to study AF-SDW singularities. On a single-layer honeycomb lattice, AF instability occurs at $U_c/t \simeq 3.6$. On a layered honeycomb lattice, inter-layer hopping term induces the fermi-surface nesting, contrary to the usual cases where three dimensionality destroys nesting behaviors. Within RPA scheme, the perfect nesting leads AF to occur at $U_c = 0$. We discuss that MgB$_2$ might be a nearly-AF metal.

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