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Stability of staggered flux state for anisotropic triangular lattice

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Abstract

In view of pseudogap-like behavior found in organic layered superconductors κ-(BEDT-TTF)$_2$X, we study the stability of correlated staggered flux state, which may bring about pseudogap behavior, with respect to the ordinary correlated Fermi sea as a low-lying normal state that underlies the unconventional superconductivity. To treat strong correlations, we apply a variational Monte Carlo method to a Hubbard model on a anisotropic triangular lattice, and construct a phase diagram of the normal state for large values of U/t. The results are qualitatively consistent with the features of non-doped κ-(BEDT-TTF)$_2$ salts.

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1. Introduction

Recent experiments on the pseudogap phase of underdoped cuprate superconductors (SC's) revealed that the origin of this phase is not a pairing fluctuation as a precursor to superconductivity (SC) but distinct magnetic orders caused by some local currents. As a possible quantum state to generate such features of the pseudogap phase, a correlated staggered flux (SF) or d-density wave state (Fig. 1(a)) [1] was recently reconsidered for the Hubbard (t-t'-U) model with plausible results [2]. Similar pseudogap-like behavior has been observed in a series of layered organic salts κ-(BEDT-TTF)$_2$X [henceforth, abbreviated as κ-(ET)$_2$X] [3-5]. Low-energy behavior of κ-(ET)$_2$X is described in most cases by the Hubbard model on an anisotropic triangular lattice at half filling [6]. The degree of

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anisotropy or frustration t'/t can be varied by substituting the anion X or by applying uniaxial pressure, and is estimated by *ab initio* calculations at 0.4-0.7 for weakly frustrated compounds and ~0.8 for a highly frustrated one κ-$(ET)_2Cu_2(CN)_3$ [5,7]. The former compounds have relatively strong antiferromagnetic (AF) correlations and bring about SC transitions at high critical temperatures as organic compounds. Among them, deuterated κ-$(ET)_2Cu[N(CN)_2]Br$ ($t'/t{\sim}0.4$) is shown to exhibit pseudogap behavior such as a steep decrease in the NMR spin-lattice relaxation time ($1/T_1T$) in the metallic phase under applied pressure. On the other hand, the latter κ-$(ET)_2Cu_2(CN)_3$, which never shows an AF order in the insulating phase under ambient pressure, exhibits a Korringa relation ($1/T_1T=$ const.) in the metallic phase under pressure down to a relatively low T_c (3-4K), namely, pseudogap behavior is missing [8]. Furthermore, similar pseudogap behavior was recently observed in a doped κ-ET salt [κ-$(ET)_4Hg_{2.89}Br_8$] [9], in which the doping rate of holes is 0.11 and $t'/t{\sim}0.8$.

In this work, we discuss the possibility that, in the anisotropic triangular lattice, SF states become stable *normal* states that underlie SC and generate the above pseudogap behavior in κ-ET salts, similarly to the case of cuprates [2]. As a method of calculation, a variational Monte Carlo (VMC) scheme is used to cope with the strong correlation.

2. Formulation

As a model of κ-ET salts, we consider a Hubbard model on an anisotropic triangular lattice (Fig. 1) [6]:

$$H=H_t+H_{t'}+H_U=-t\sum_{\langle i,j\rangle\sigma}\left(c_{i\sigma}^\dagger c_{j\sigma}+\mathrm{H.c.}\right)-t'\sum_{(i,j)\sigma}\left(c_{i\sigma}^\dagger c_{j\sigma}+\mathrm{H.c.}\right)+U\sum_j d_j\ , \tag{1}$$

where $d_j=n_{j\uparrow}n_{j\downarrow}$, $n_{j\sigma}=c_{j\sigma}^\dagger c_{j\sigma}$, and the sums of $\langle i,j\rangle$ and (i,j) are taken for nearest-neighbor pairs and for diagonal-neighbor pairs in the (1,1) and $(-1,-1)$ directions, respectively; thus, the energy dispersion of the noninteracting part is given by $\tilde{\varepsilon}_{\mathbf{k}}=-2t\left(\cos k_x+\cos k_y\right)-2t'\cos\left(k_x+k_y\right)$. In this model, we study the stability of the correlated staggered flux state $\Psi_{\rm SF}=P\Phi_{\rm SF}$ with respect to the ordinary projected Fermi sea ($\Psi_{\rm N}=P\Phi_{\rm N}$) as a normal state underlying the SC state. Here, P is a product of many-body factor discussed shortly. The one-body function $\Phi_{\rm SF}$ is the ground state of a non-interacting staggered flux Hamiltonian $H_{\rm SF}$ in each plaquette of which a magnetic flux of $\pm 4\theta$ penetrates alternately (Fig. 1(a)). Because of the band folding by (π,π), $\Phi_{\rm SF}$ is given as a mixed state of the operators of the two sublattices with θ being a variational parameter here:

$$\Phi_{\rm SF}=\prod_{\mathbf{k}\in\mathbf{k}_{\rm F},\sigma}\frac{1}{\sqrt{2}}\left[\gamma_{\mathbf{k}}(\theta)c_{\mathrm{A}\mathbf{k}\sigma}^\dagger+c_{\mathrm{B}\mathbf{k}\sigma}^\dagger\right]|0\rangle\ ,\qquad c_{\Lambda j\sigma}=\sqrt{\frac{2}{N_{\rm s}}}\sum_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{r}_j}c_{\Lambda\mathbf{k}\sigma}\ , \tag{2}$$

where A (B) labels the sublattice, $\Lambda=\mathrm{A}$ or B, and $\gamma_{\mathbf{k}}(\theta)=2te^{ik_x}\left(e^{i\theta}\cos k_x+e^{-i\theta}\cos k_y\right)/|E_-^{\rm SF}(\mathbf{k})|$. Here, $E_-^{\rm SF}(\mathbf{k})=-\sqrt{(1+\cos 2\theta)/2}\sqrt{\varepsilon_{\mathbf{k}}^2+\Delta_{\mathbf{k}}^2}$ is the energy dispersion of the lower band for $H_{\rm SF}$ with $\varepsilon_{\mathbf{k}}=-2t\left(\cos k_x+\cos k_y\right)$, $\Delta_{\mathbf{k}}=\Delta_\theta\left(\cos k_x-\cos k_y\right)$, and $\Delta_\theta=2t\sqrt{(1-\cos 2\theta)/(1+\cos 2\theta)}$. Note that $E_-^{\rm SF}(\mathbf{k})$ has a form ($d_{x^2-y^2}$-wave gap) similar to the quasiparticle energy in d-wave SC, and its band top forms a Dirac cone centered at $(\pi/2,\pi/2)$ for the π-flux case ($\theta=\pi/4$). For $\theta<\pi/4$, the Dirac cone is elongated in the $(\pi,0)$-$(0,\pi)$ direction. In a doped case, the Fermi surface is made of a cross section of this elongated Dirac cone, which resembles a Fermi arc observed for cuprates by ARPES etc. $\Phi_{\rm SF}$ breaks the lattice rotational, lattice translational and time reversal symmetries. To $\Phi_{\rm SF}$, we multiply correlation factors, $P=P_{\rm G}(g)P_Q(\zeta_{\rm d},\zeta_{\rm h})\,P_\phi(\phi)$. Here, $P_{\rm G}(g)$ is the onsite (Gutzwiller) projection, and $P_Q(\zeta_{\rm d},\zeta_{\rm h})$ a nearest-neighbor doublon-holon projection indispensable for treating Mott physics [10,11]. In addition to these two, we have to include a configuration-dependent phase factor P_ϕ required by Mott physics for a current-carrying state [12,2]. In the present case, an appropriate form of P_ϕ is given by,

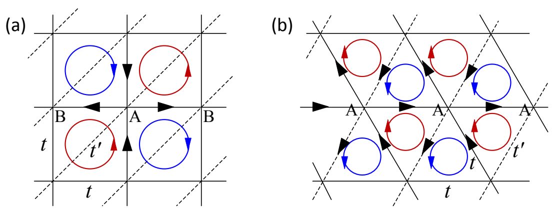

Fig. 1. (a) Schematic figure of staggered current in square plaquettes in $\Psi_{\rm SF}$. The characters A and B indicate the sublattices; (b) the same in triangular plaquettes in $\Psi_{\rm tri}$. Every lattice point is equivalent (A). The arrows on the lattices in both panels indicate the direction of Peierls phases θ.