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LETTER TO THE EDITOR

The ordered phase of electron vortices

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Abstract. Stability conditions for the ordered state of the magnetic fluxes induced by rotating electrons on a square lattice are analysed in the mean-field approximation for the extended Hubbard model. It is shown that the flux phase can appear if the exchange energy V_1 is sufficiently large. The order parameter, magnetic flux Φ enclosed in the unit cell, and critical temperature of the flux phase are monotonically increasing functions of V_1. It is also shown that the flux and the antiferromagnetic phase can coexist.

A few years ago Fisher and Fradkin [1], when analysing a 2D tight-binding model of electrons in a magnetic field, realised that in the case when the magnetic flux per plaquette Φ of a square lattice is equal to $hc/2e$ time-reversal invariance is not truly broken. There is no difference in the physics for the system with the flux $+\Phi$ and $-\Phi$. The system has a semi-metallic band structure. Recently the problem reappeared together with new concepts of superconductivity [2]. The authors [2] considered a strongly correlated electron system in the framework of a pure exchange model (called also the t–J model), which is a canonical transformation of the Hubbard model in the limit of the large on-site Coulomb energy U_0. Using a slave-boson formalism it was shown that in the system with the average number of electrons $\bar{n} = 1$ per site, besides the superconductivity there is a flux phase with the fluxes $\Phi = \pm hc/2e$ ordered as a chess-board.

It is surprising that the authors [1, 2] analysed the ordered flux state only with the flux Φ equal to $hc/2e$. Is it not possible that there is a flux state with another value of Φ? The flux Φ, as the order parameter, should be dependent on interactions in the system as well as on temperature. The purpose of the present work is to investigate this problem in the framework of the extended Hubbard model, which is richer than the t–J model. This should enable us to understand the role of the exchange process for stability of the flux phase. Besides the flux state the magnetic and the charge density orderings are analysed.

I start with the description of the considered model. It is a two-dimensional tight-binding model of electrons on a square lattice. Its Hamiltonian has the form

$$H = \frac{t}{2}\sum_{\substack{i,\delta\\ \sigma}} c_{i\sigma}^{+}c_{i+\delta\sigma} + U_0\sum_{i,\sigma} c_{i\sigma}^{+}c_{i\sigma}c_{i-\sigma}^{+}c_{i-\sigma} + \frac{U_1}{2}\sum_{\substack{i,\delta\\ \sigma,\sigma'}} c_{i\sigma}^{+}c_{i\sigma}c_{i+\delta\sigma'}^{+}c_{i+\delta\sigma'} + \frac{V_1}{2}\sum_{\substack{i,\delta\\ \sigma}} c_{i\sigma}^{+}c_{i+\delta\sigma}c_{i+\delta-\sigma}^{+}c_{i-\sigma}. \tag{1}$$

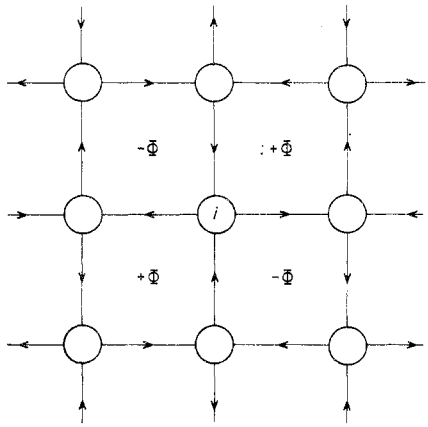

Figure 1. The system under consideration—electron vertices periodically ordered on a square lattice. Φ denotes the magnetic flux, which is induced by a rotating current around the plaquette.

Here, $c_{i\sigma}$ denotes an annihilation operator of an electron with spin $\boldsymbol{\sigma}$ ($\boldsymbol{\sigma} = +, -$ for the spin up and down) at the site i, $\boldsymbol{\delta}$ is the vector to the nearest-neighbour site. The first term describes hopping of electrons, the second term the interactions of two electrons with the opposite spins at the same site, and the two last terms describe the Coulomb and exchange interactions of two electrons at the nearest-neighbour sites. The parameters corresponding to these processes are: the hopping integral t, which is taken as $t = -1$ in our calculations; the Coulomb integrals U_0, U_1 for electrons at the same site and the nearest-neighbour site, respectively; and V_1 is the exchange integral.

It is assumed that there are local-electron currents, each rotating around the plaquette of four bonds. Moreover, the electron vortices are periodically ordered. Since rotating electrons induce local magnetic fields, one can make predictions about periodically ordered phases of magnetic fluxes. The flux for each plaquette is $\pm\Phi$. Such a situation is exhibited in figure 1. The order parameter for the flux phase may be defined as

$$\begin{aligned} \langle c^+_{i\sigma} c_{i\pm x\sigma}\rangle &= n_1 \exp[\mathrm{i}\varphi \cos(\boldsymbol{Q}\cdot\boldsymbol{R}_i)] \\ \langle c^+_{i\sigma} c_{i\pm y\sigma}\rangle &= n_1 \exp[-\mathrm{i}\varphi \cos(\boldsymbol{Q}\cdot\boldsymbol{R}_i)] \end{aligned} \tag{2}$$

where $\varphi = \pi\Phi/(2\Phi_0)$, $\Phi_0 = hc/e$ is a one-electron flux quantum, the wavevector $\boldsymbol{Q} = (\pi/a, \pi/a)$, and a is the lattice constant. This definition is consistent with the law of current conservation (Kirchhoff's law) at each site. One can also consider the antiferromagnetic (AF) and the charge-density (CDW) ordering defined by

$$m_i = \sum_\sigma \sigma \langle c^+_{i\sigma} c_{i\sigma}\rangle = m_0 \cos(\boldsymbol{Q}\cdot\boldsymbol{R}_i), \tag{3}$$

$$n_i = \sum_\sigma \langle c^+_{i\sigma} c_{i\sigma}\rangle - \bar{n} = n_0 \cos(\boldsymbol{Q}\cdot\boldsymbol{R}_i). \tag{4}$$

We assume that the average number of electrons per site is given by

$$\bar{n} = \frac{1}{N}\sum_{i,\sigma} \langle c^+_{i\sigma} c_{i\sigma}\rangle = 1 \tag{5}$$

where N denotes the number of the sites in the system.

We can rewrite the Hamiltonian (1) in the mean-field approximation as

$$H_{\mathrm{MF}} = -\sum_{k,\sigma} \eta_k [1 - n_1(V_1 - U_1)\cos\varphi] c^+_{k\sigma} c_{k\sigma} + \sum_{k.\sigma} [-\sigma m_0 U_0 + n_0(U_0 + U_1) + \mathrm{i} n_1 (V_1 - U_1)\gamma_k \sin\varphi] c^+_{k\sigma} c_{k+Q\sigma} \tag{6}$$

where

$$\eta_k = \cos k_x a + \cos k_y a$$
$$\gamma_k = \cos k_x a - \cos k_y a.$$

Here $\boldsymbol{k} = (k_x, k_y)$ is the wavevector of an electron. One can easily diagonalise the Hamiltonian (6) and find the stability conditions for the AF, CDW and flux phases (FL) at the temperature T

$$1 = U_0 \frac{1}{8\pi^2 a^2} \int\int \frac{\tanh(\beta E_k/2)}{E_k} \mathrm{d}k_x \, \mathrm{d}k_y \quad (\mathrm{AF}) \tag{7}$$

$$1 = (-U_0 - U_1) \frac{1}{8\pi^2 a^2} \int\int \frac{\tanh(\beta E_k/2)}{E_k} \mathrm{d}k_x \, \mathrm{d}k_y \quad (\mathrm{CDW}) \tag{8}$$

$$\left.\begin{aligned} 1 &= (V_1 - U_1) \frac{1}{8\pi^2 a^2} \int\int \gamma_k^2 \frac{\tanh(\beta E_k/2)}{E_k} \mathrm{d}k_x \, \mathrm{d}k_y \\ n_1 \cos\varphi &= [-1 + n_1(V_1 - U_1)\cos\varphi] \frac{1}{8\pi^2 a^2} \int\int \eta_k^2 \frac{\tanh(\beta E_k/2)}{E_k} \mathrm{d}k_x \, \mathrm{d}k_y \end{aligned}\right\} (\mathrm{FL}) \tag{9}$$

where

$$E_k = \{\eta_k^2 [1 - n_1(V_1 - 2U_1)\cos\varphi]^2 + [m_0 U_0 + n_0(U_0 + U_1)]^2 + n_1^2 (V_1 - U_1)^2 \gamma_k^2 \sin^2\varphi\}^{1/2}$$

and $\beta = 1/k_{\mathrm{B}}T$. The integration is over the first Brillouin zone. It is seen that all integrals are positive and thus, the AF and CDW phases are stable if $U_0 > 0$ and $U_0 + U_1 < 0$, respectively. The flux phase is stable for $V = V_1 - U_1 > 0$. The conditions (7) and (8) are the same if one exchanges the parameters U_0 and $-U_0 - U_1$. Therefore, we consider only the AF phase and the flux phase. The first integration in equations (7)–(9) gives the elliptic integrals of the first and second kinds. The second integration is performed numerically. (Only in the extreme cases, for small parameters U_0 and V, was it not possible to determine these singular integrals.)

Figure 2 presents the stability regions for the antiferromagnetic and the flux phase in the plane of the parameters U_0 and $V = V_1 - U_1$. The AF and the FL states are stable along the vertical and the horizontal axis, for any $U_0 > 0$ and $V > 0$, respectively. These phases are separated by the wide region of the mixed phase (FL + AF), where both order parameters are $\Phi > 0$ and $m_0 > 0$.

Figure 3 presents the dependence on the parameter V of the order parameters, the magnetic flux Φ and n_1 for the FL phase, as well as the local magnetisation m_0 for the AF ordering for two values of U_0 ($U_0 = 0$, (curves A), and $U_0 = 2$ (curves B)). It is seen that Φ is a monotonically increasing function of V. At $U_0 = 0$ the parameter n_1 increases slightly for small V and decreases for higher values of V. The AF ordering, with the magnetisation $m_0 > 0$, appears at a finite value of the on-site Coulomb integral U_0

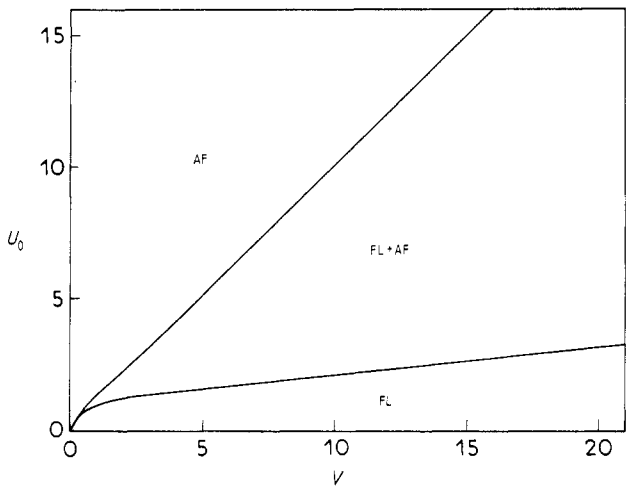

Figure 2. Stability regions of the antiferromagnetic phase (AF), the flux phase (FL), and the mixed (flux–antiferromagnetic) phase (FL + AF) in the plane of parameters U_0 and $V = V_1 - U_1$ for a square lattice with the average number electrons $\bar{n} = 1$ per site.

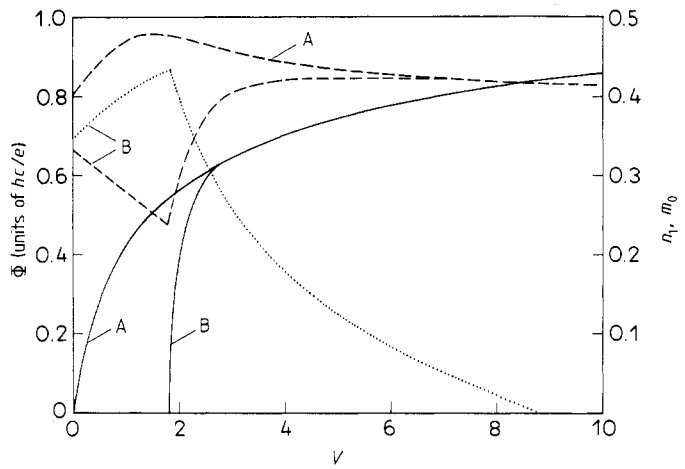

Figure 3. Dependence on $V = V_1 - U_1$ and the order parameters: Full curve, flux, Φ; broken curve, n_1; dotted curve, magnetisation, m_0 for $U_0 = 0$ (curves A) and $U_0 = 2$ (curves B) at $T = 0$.

and at small V. The order parameter m_0 increases with V, whereas the parameter n_1 decreases. In the mixed phase m_0 is strongly damped with the increasing V. For very large V only the flux states exist.

In figure 4 the temperature dependence of the order parameters Φ, n_1 and m_0 for $V = 2.5$, and $U_0 = 0$, 2 and 3 (curves A, B and C) is exhibited. Curves A correspond to the case when only the FL phase exists, curves C to the AF phase. In general, all parameters are temperature dependent. However, in the AF phase (curve C) the parameter $n_1(T)$ increases only slightly, and the magnetisation $m_0(T)$ has a typical mean-field characteristic. For case 2 (curve B: $U_0 = 2$, $V = 2.5$) the mixed phase exists. The analysis showed that the critical temperature T_{AF} (for the AF ordering) is always lower

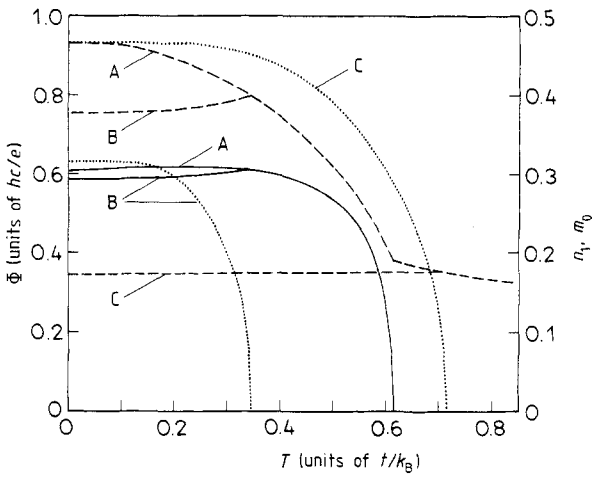

Figure 4. Temperature dependence of: full curve, flux Φ; broken curve, n_1; dotted curve, magnetisation, m_0 for $U_0 = 0$ (curves A), $U_0 = 2$ (curves B) and $U_0 = 3$ (curves C). All curves are at $V = 2.5$. The temperature T is in units t/k_B.

than the critical temperature T_{FL} (for the FL ordering). A decrease of the magnetisation m_0 with T causes an increase of Φ and n_1.

In conclusion, the flux phase induced by electron current vortices may appear in the system with a large exchange energy. It is not restricted to the extended Hubbard model, but may also occur in the t-J model. In contrast to the previous works [1, 2], it has been shown that the flux Φ per plaquette is a monotonic function of the exchange parameter V as well as the temperature. The on-site Coulomb energy U_0 stabilises the AF ordering and destroys the flux phase. However, there is a wide region of parameters where the FL and the AF phases (or the FL and the CDW phases) coexist. The present considerations were made in the mean-field approximation. One can expect that fluctuations, which are important in 2D systems, lead to another ground state. Introduction of some additional charges into the system (deviation from $\bar{n} = 1$) destabilise the ordered flux phase. The more favourable phase, in such a case, may be a liquid state of fluxes with some topological defects (e.g. skyrmions). It is interesting to investigate the flux phase in the presence of superconductivity, when the Cooper pairs have a non-zero orbital moment and when they induce local magnetic fields (local fluxes). These problems are under consideration and will be presented in the near future.

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