"Broken strings": Unidirectional and double self-trapping of charge carriers in antiferromagnetic semiconductors

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If the checkerboard ordering in a Hubbard antiferromagnetic semiconductor is replaced by layering, a self-trapped charge-carrier state changes from a magnetic string to a new state. In this state a carrier is self-trapped in one direction while remaining free in the others (a "broken string"). Close to the boundary between these two antiferromagnetic phases the energy of a broken string is lower than that of an ordinary string. Hence regions of the stratified phase can develop inside the checkerboard phase. They are stabilized by trapping broken strings inside them (double self-trapping).

As is well known, magnetic self-trapping of the charge carriers is characteristic of antiferromagnetic semiconductors (see my earlier monograph[1] and review[2]). It is now widely recognized that this phenomenon may be connected with high-temperature superconductivity. The concept of heterophase self-trapping was introduced in Ref. 3: a carrier creates a microregion of a different phase, which it stabilizes by being trapped inside it. The case treated in Ref. 3 corresponds to carrier trapping inside a ferromagnetic region. I called such a quasiparticle a "ferron." In Ref. 4 carrier trapping takes place in an antiferromagnetic region of a kind different from the original one. This type of quasiparticle is called an afmon. States corresponding to heterophase self-trapping can occur when the magnet spin exceeds 1/2, but they are completely impossible in Hubbard models.[2]

On the other hand, in such models very different kinds of carrier states are possible, in which no regions containing a new phase develop. The first example of this type was given by Bulaevskiĭ *et al.*[5] The corresponding quasiparticle, called a quasi-oscillator in Ref. 5, is now usually referred to in the literature as a magnetic string. It arises in antiferromagnets with checkerboard ordering, and is characterized by charge carriers (e.g., conduction electrons) that oscillate about an equilibrium position that moves slowly through the crystal. When an electron leaves the equilibrium position, a chain of reversed spins develops along its trajectory, corresponding to antiphase antiferromagnetic ordering along its trajectory. When the electron returns to equilibrium along the same trajectory, it destroys the antiphase ordering, and normal antiferromagnetic ordering is restored. As was shown in Refs. 6 and 7, strong pairing can give rise to HTSC.

But this kind of string cannot occur in Hubbard models describing antiferromagnetic materials with different kinds of ordering, e.g., Landau stratification. This case is the one which we investigate here. Its distinguishing feature is that the motion of a conduction electron in the direction perpendicular to the ferromagnetic layers induces spin reversal, while motion parallel to the layers does not. For this reason, chains of reversed spins along electron trajectories are found to broken, so we will call the corresponding carrier state a broken carrier string. The main difference between this state and states previously known is that the electron is self-trapped in only one direction (perpendicular to the magnetic layers) and remains free in the other directions. This is a nontrivial situation. For example, in ferron and afmon states, even if the antiferromagnetic ordering is stratified the electron remains self-trapped in all directions, including the direction parallel to the ferromagnetic layers.

Near the boundary between the checkerboard and stratified antiferromagnetic phases the string energy in the stratified phase should be less than in the checkerboard phase (see below). Consequently, a new phenomenon, double self-trapping, is possible. It consists of the following: On the side of the interphase boundary where the checkerboard phase is stable, regions of the stratified phase containing strings can occur. Thus, current carriers that are already present in self-trapped magnetic string states undergo additional heterophase self-trapping. In other words, in contrast to the treatment of Refs. 3 and 4, the regions of stratified phase here arise as a result of self-trapping not of the free current carriers, but of the already self-trapped electrons and holes.

In degenerate semiconductors it is possible to have a situation in which a crystal decays into regions of the checkerboard and stratified phases, such that each region of the stratified phase contains many electrons at one time. In contrast, at $T=0$ there are no conduction electrons in the stratified phase. This process, which Emery *et al.*[8] call phase separation, was first studied by Nagaev[9] in connection with the *s–d* model for the case in which the highly conductive phase is ferromagnetic and the insulating phase is antiferromagnetic. The process was studied in a very model-dependent fashion in Ref. 8, where it was found that an antiferromagnetic Hubbard semiconductor can be separated into antiferromagnetic and nonmagnetic phases. Nagaev and Podel'shchikov[10] used the *s–d* model to study the separation of a degenerate antiferromagnetic semiconductor into checkerboard and stratified phases. The difference between the situation here and that in Refs. 9 and 10 is that here the new phase is created not by free charge carriers, but by strings. But it also differs from the situation

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studied in Ref. 8, not only in the nature of the phases but also in the small number of carriers in the calculation per magnetic atom in the highly conductive phase, which eliminates the possibility of Coulomb disruption of the crystal in states with separated phases.

In the present work we report a calculation only of the one-electron problem. As in Ref. 5 we will use the t–J model, and for simplicity we will take the crystal to have a simple square lattice. To ensure the stability of the stratified phase in this structure it is necessary to take into account the exchange integrals J_1 and J_2 between the nearest and next-nearest neighbors respectively. The boundary between the checkerboard and stratified phases is determined by the condition $J_1=2J_2<0$ (the stratified phase is stable for even smaller J_2). The wave function of a stationary string, just as in Ref. 5 for the checkerboard phase, is found for the stratified phase by expanding over all electron trajectories, starting from the equilibrium point $\mathbf{g}$. Its form differs from that of Ref. 5, however, because account is taken of the conservation of the projection of the atomic spin when a conduction electron (i.e., the second electron on an atom) moves parallel to the ferromagnetic layers, which are perpendicular to the x axis:

$$\psi(\mathbf{g})=\sum_{n=0}^{\infty}\sum_{\Delta}c(\mathbf{g},\Delta_1,\ldots\Delta_n)(S_{\mathbf{g}}^{-})^{d_1}\cdots \times(S^{-}_{\mathbf{g}+\Delta_1+\ldots\Delta_{n-1}})^{d_n}p^{*}_{\mathbf{g}+\Delta_1+\ldots\Delta_n}|0\rangle, \tag{1}$$

where Δ inside the sigma represents summation over all vectors Δ_i connecting nearest neighbors under the restriction $\Delta_n\neq-\Delta_{n+1}$. The symbol d_n stands for $|\Delta_n^x|$, we have written $S^{-}=S^{x}-iS^{y}$, and $p_{\mathbf{f}}^{*}$ is the pair creation operator for holes with opposite spins at an atom with index $\mathbf{f}$. The vacuum wave function $|0\rangle$ describes the state with one electron per atom when the atomic spins are ordered antiferromagnetically so that the ferromagnetic "layers" are parallel to the y axis.

The vacuum wave function does not include zero spin oscillations. This approach is justified for Ising systems in any case. As for Heisenberg systems, it is felt that in the two-dimensional case the zero spin oscillations have so large a role that these systems can be in a spin liquid state rather than an antiferromagnetic state. Although the final answer to this question remains unknown, it is clear that the approximation used here is reasonable, at least for three-dimensional systems. In the case of Heisenberg systems, the wave function (1) shows that, in accordance with the condition that the electron transition integral between atoms is large compared with the exchange integrals, the spins of the magnetic atoms do not change over the time required by an electron to traverse several lattice constants.

Using (1) and making use only of the strong inequality $|B|\gg|J|$, where B is the Bloch integral for nearest neighbors, it can easily be found to this approximation that the wave function has the following form:

$$Ec(\mathbf{g})=B\sum_{\Delta}c(\mathbf{g},\Delta), \tag{2}$$

$$[E-K(\Delta_1,\ldots,\Delta_n)]c(\mathbf{g},\Delta_1,\ldots,\Delta_n)=B\sum_{\Delta_{n+1}}c(\mathbf{g},\Delta_1,\ldots\Delta_n,\Delta_{n+1}) \tag{3}$$

with

$$c(\mathbf{g},\Delta_1,\ldots,\Delta_n,\Delta_{n+1},-\Delta_{n+1})=c(\mathbf{g},\Delta_1,\ldots,\Delta_n). \tag{4}$$

The diagonal matrix elements of the Hamiltonian are linear in J_1 and J_2. Their dependence on Δ is fairly complicated, but it can be approximated as follows:

$$K(\Delta_1,\ldots,\Delta_n)\approx k\sum_{i=1}^{n}d_i, \tag{5}$$

$$k=6|J_2|S^2,\quad S=1/2. \tag{6}$$

Using this representation we can find the energy of the ground state of a string by substituting

$$c(\mathbf{g},\Delta_1,\ldots,\Delta_n)=\varphi\Big(\sum_{i=1}^{n}d_i\Big). \tag{7}$$

From Eqs. (5)–(7) we can derive the following equation for a broken string using the effective-mass approximation:

$$E_{ts}\varphi(x)=Fx\varphi(x)-\frac{1}{2m}\frac{d^2\varphi}{dx^2},\quad(\hbar=1), \tag{8}$$

$$E_{ts}=E+4|B|,\quad F=k/a,\quad 1/2m=|B|a^2, \tag{9}$$

with the boundary condition

$$a^2b\varphi'(0)+\varphi(0)=0, \tag{10}$$

$$b=(2mF)^{1/3}, \tag{11}$$

where a is the lattice constant. The eigenfunction of Eqs. (8)–(10) is an Airy function:

$$\varphi(x)=\mathrm{Ai}(z),\quad z=b(x-E_{ts}/F). \tag{12}$$

From Eqs. (10)–(12) and the condition $|J_2/B|\ll1$ the energy of a broken string is given by

$$E=-4|B|+Fu/b, \tag{13}$$

where $u\approx2.4$ is the smallest root of the Airy function.

As for the width of the band of a string, corresponding to the translational motion through the crystal of its equilibrium position, two factors determine it in the case of checkerboard ordering:[11] the trajectories with self-intersection, and the zero spin oscillations. (Trugman[12] later reached a similar conclusion.) In the present instance the motion of a string parallel to the ferromagnetic layers is equivalent to the motion of a free quasi-particle. But the motion is very different in the perpendicular direction. I was unable to find any trajectories giving rise to motion in this direction. Thus, it is reasonable to assume that the motion here is determined by the zero spin oscillations. This means that the corresponding component of the effective mass tensor of the string must be of the same order of magnitude as that found in Ref. 11 for the checkerboard case. The latter was typically found to be on the order of the magnon effective mass, i.e., larger by a factor of B/J than the effective mass component parallel to the layers.

In order to compare the energies of a normal string in the checkerboard case and a broken string in the stratified case, the results[5,11,13] obtained for the former in the nearest-neighbor exchange approximation should be generalized to the case in which the exchange interactions between next-nearest and next-next-nearest neighbors are also important. Close to the phase boundary the expression for the string energy in the checkerboard phase differs from (13) in having the factor v in place of u. Both are of order unity, but the exact value of v is unknown. We can say, however, that v is larger than u. This follows from the obvious fact that as $|J_2|$ increase without bound the energy of a normal string approaches zero, while that of a broken string approaches $-2|B|$.

The fact that the energy of a string in the stratified phase is lower than in the checkerboard phase implies that heterophase self-trapping of a string is possible, accompanied by transformation from the normal to the broken form. If the checkerboard phase is stable in the absence of carriers, but the difference $D=2J_2-J_1$ is small, then inside the checkerboard phase there should be regions of the stratified phase containing broken strings. It is natural to assume that they have rectangular shape with sides X and Y.

The optimum dimension X in the direction perpendicular to the ferromagnetic layers should be of order b^{-1}. Specifically, for $X \ll 1/b$ the string is located primarily outside the region of stratified ordering, so that its energy is close to that of a normal string. On the other hand, if $X \gg 1/b$ holds it is easy to show by using the asymptotic expression for $\mathrm{Ai}(x)$ and $\mathrm{Bi}(x)$, the Airy functions of the first and second kind, that the size-dependent correction to the energy of a broken string is a quantity of order $\exp[-(4/3)(Xb)^{2/3}]$. It can therefore be neglected for $Xb > 2$. For this reason we must set X approximately equal to $2/b$ when D is very small. Then the energy of a self-trapped broken string should be determined from the condition for the minimum energy,

$$E=2DXYa^{-2}+\pi^2/2mY^2+F(u-v)/b, \tag{14}$$

which in the limit $D\to 0$ yields a further reduction in the energy of a normal string by a quantity of order F/b, with

$$(Y/a)^{1/3}\sim |B/D|. \tag{15}$$

Analogous expressions for the ferron and afmon dimensions in the two-dimensional case show that when the cost D of creating a new phase is the same, the number of atoms in it for those quasiparticles is larger than for a broken string. It is significant that double self-trapping causes the unidirectional self-trapping typical of a broken string to be transformed into self-trapping in all directions.

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