Aspects of d-Density Order*

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ABSTRACT

I briefly review the concept of d-density ordering, extend it to arbitrary dimensions, and speculate that it might describe Mott insulators. This ordering supports zero modes on domain walls, and quite plausibly dopants occupy such states. This phenomenon could induce quasi-one dimensional behavior in a two-dimensional electron system.
In this talk I will briefly describe some recent and ongoing work done in collaboration with Chetan Nayak [1, 2].

1. Introduction

One has become accustomed to the existence of subtle ordering in particle-particle channels, especially in connection with the superfluidity of $^3$He, and also in the apparent d-wave superconductivity of cuprates and the less certainly determined, but apparently non-s wave, pairings for heavy fermion systems. On the other hand several familiar types of ordering, including spin-density wave (and thus ferromagnetic and antiferromagnetic, among others) and charge-density wave, can be described as pairing in particle-hole channels. It is therefore interesting to inquire whether orderings involving more subtle particle-hole pairings occur naturally – in models, and in reality – and if so, whether they might have important physical consequences.

Here I will discuss a particular example of such ordering, which for reasons that will become apparent we call d-density ordering. I will show that it appears very naturally in a simple model of considerable physical interest, and that both the ground state and the quasiparticles have quite interesting properties, suggesting that this type of ordering may have something to say about the Mott insulator phenomenon. In this connection it is particularly interesting that the quasiparticles plausibly are localized on domain walls. That association provides a natural mechanism whereby quasi-one dimensional dynamics could govern interactions among the quasiparticles in a two dimensional system.
2. Ground State; Symmetry Properties

In [1] we arrived at the possibility of a new kind of ordering by studying a particular model Hamiltonian; here I shall instead first define the ordering in a general way, and only then discuss its dynamical origin. Consider a two-dimensional square lattice with spacing \( a \), aligned along the coordinate axes. It is natural, for several reasons, to consider symmetry breaking at momentum \( G/2 \equiv (\frac{\pi}{a}, \frac{\pi}{a}) \). Indeed, ordering at such a momentum – half a reciprocal lattice vector – can be induced by quartic interactions at the mean-field level, as we shall discuss concretely in a moment. Well-established possibilities, including antiferromagnetic and commensurate charge-density order are described in this way. Also in two dimensions this momentum vector has a special significance, since the tight-binding Fermi surface nests here at half filling. The d-density order is characterized abstractly by the expectation value

\[
\langle c_{k+G/2}^{\dagger} c_k \rangle = i \delta_{\alpha \beta} f(k).
\]

Here \( \alpha, \beta \) are spin indices, and \( f \) is a real function that changes sign upon rotation by \( \pi/2 \). The ordering defined by (2.1) breaks three important symmetries:

- Translation by one lattice spacing (because of the momentum transfer \( G/2 \)).

- Time reversal symmetry, as suggested by the appearance of \( i \).

- The discrete rotation through \( \pi/2 \).

However the square of these operations, or any product of any two of them, is a valid symmetry. There is no macroscopic T violation, therefore. The broken symmetry is parametrized by the simplest of all groups, \( Z_2 \).
Because one obtains the true density by integrating (2.1) over $k$ there is a cancelation, and the charge distribution is homogeneous. However the ordering in its mathematical form does resemble a d-wave analogue of a charge density wave, which explains the name. There is also the possibility of d-spin density wave ordering, but I will not discuss that further here. Our d-density order parameter, of course, is a spin singlet.

One can also discuss the ordering in real-space terms. The relevant vacuum expectation value is of the form

$$\text{Im} \langle c^\dagger_\alpha(x + a\hat{n})c_\beta(x) \rangle = \delta^\alpha_\beta g(x)$$

where $g$ is a real function that changes sign upon translation by a minimal lattice vector, and $\hat{n}$ is a unit vector along a coordinate axis. In this form we see some similarity between d-density ordering and staggered flux phases. In fact microscopic currents do flow in the d-density ground state; however their value does not correspond to any simple value of the flux (e.g. 0, $\pm\pi/2$, $\pi$).

Upon d-density ordering the effective size of the unit cell is doubled, and thus a gap opens at half filling. The Mott insulator phenomenon, in its most basic form, is therefore an automatic consequence.

For definiteness I have in the preceding supposed 2-dimensional kinematics, however let me emphasize that the concepts extend in a most natural way to other dimensions. Above, I have taken care to formulate them in such a way that the extension is obvious (this may not have not been transparent in [1]).

To judge the physical reasonableness of d-density order we must consider whether it arises in the ground state of some simple, significant Hamiltonian.

Though in some sense it is a case of “old wine in new bottles”, we think it is quite noteworthy and remarkable that the 1-dimensional version arise for the very simplest Hubbard model at half filling. This is most easily seen upon bosonizing the theory. The analysis is detailed in [2]; here I shall be very telegraphic. The
Fermi surface splits into two points, describing left- and right-movers. Spin and charge excitations travel at different velocities, and are conveniently represented by different fields. Let the charge field for left and right movers be represented by the appropriate components $\chi_{L,R}$ of a scalar field $\chi$ compactified on a circle of radius $1/\sqrt{2}$. At generic values of the filling, these are free fields. Precisely at half filling there is an additional relevant interaction, the Umklapp process, that in terms of the electron fields is

$$L_{\text{umklapp}} = u(\epsilon_{\alpha\beta}\psi^\dagger_L \psi^\dagger_R)(\epsilon^{\gamma\delta}\psi_R \psi_L)$$  \hspace{1cm} (2.3)$$

and for the holon fields induces the simple form

$$L = \frac{1}{2} (\partial \chi)^2 + 2u \cos \sqrt{2}\chi .$$  \hspace{1cm} (2.4)$$

Here $\chi \equiv \chi_L + \chi_R$ and $u = \frac{U}{16t}$, where $t$ is the hopping parameter. This holon Lagrangian is invariant under the $Z_2$ symmetry $\chi \rightarrow -\chi$ which interchanges the two Fermi points. For an attractive interaction $u < 0$ the energy is minimized at $\langle \chi \rangle = 0$, and for a repulsive interaction $u > 0$ the energy is minimized at $\langle \chi \rangle = \pi/\sqrt{2}$. In the latter case the $Z_2$ symmetry is broken.

In terms of the holon variables $\psi_L \equiv e^{-i\chi/\sqrt{2}}$, $\psi_R \equiv e^{i\chi_R/\sqrt{2}}$, $\langle \chi \rangle = 0$ corresponds to

$$\langle \psi_R \psi_L^\dagger \rangle = \langle \psi_L \psi_R^\dagger \rangle = c ,$$

a real number. This is a conventional, commensurate charge density wave. On the other hand $\langle \chi \rangle = \pi/\sqrt{2}$ corresponds to

$$\langle \psi_R \psi_L^\dagger \rangle = -\langle \psi_L \psi_R^\dagger \rangle = if ,$$  \hspace{1cm} (2.5)$$

a pure imaginary number. As a result of the minus sign this state does not have charge-density order, contributions from L-R and R-L terms canceling. Instead, (2.5) is precisely of the d-density form.
In [1] we analyzed a two-dimensional generalized Hubbard model with interaction Hamiltonian
\[ H_{\text{int.}} = U \sum_x c_{\uparrow}^\dagger(x) c_{\downarrow}^\dagger(x) c_{\downarrow}(x) + \frac{1}{2} V \sum_{x,x'} c_{\alpha}^\dagger(x) c_{\alpha}(x) c_{\beta}^\dagger(x') c_{\beta}(x') \] (2.6)
containing both on-site and nearest neighbor repulsion. We found that d-density order is plausibly the ground state for a range of \( U \) and \( V \) around \( U \approx 4V \) near half filling. This was done by considering BCS-like trial wave functions of the form
\[ \Psi = \prod_k (u_{k\uparrow} c_{k\uparrow}^\dagger + v_{k\uparrow} c_{k+G/2\downarrow}^\dagger) (u_{k\downarrow} c_{k\downarrow}^\dagger + v_{k\downarrow} c_{k+G/2\uparrow}^\dagger) |0> , \] (2.7)
and minimizing the energy as a function of the \( u_k, v_k \) (subject of course to \( |u_k|^2 + |v_k|^2 = 1 \)). The interaction energy that drives one toward d-density order arises entirely from the \( V \) term. Note that away from perfect nesting the transition occurs at a finite coupling.

3. Quasiparticles on Domain Walls?

In the previous section, I have described a form of \( Z_2 \) symmetry breaking that opens up a gap at half filling. With a \( Z_2 \) symmetry breaking, there is the possibility of domain walls marking the boundary between the different phases. In different languages and in various contexts (see for example [3, 4, 5, 6]), it is known that in this kind of situation there is a very interesting dynamical possibility associated with the domain walls. The particles which acquire mass from the transition will have a positive mass on one side and a negative mass on the other. Normally of course in a homogeneous phase we can define the negative mass away, but here the relative sign is important. It leads to the formation of zero-modes. In the present context, this means that there are mid-gap excitations localized to such walls.

It is quite conceivable that in the presence of d-density order the most favorable way to accommodate electrons doped away from half filling is to associate them
with pre-existing domain walls, or even that such particles spontaneously nucleate wall-bits (very much in the spirit of the “SLAC bag” [4]). In one dimension this is the case: charged excitations are associated with solitons of the sine-Gordon model (2.4).

Whenever it occurs, the dynamical consequences of localizing dopants to domain walls are sure to be profound. For example, in two dimensions the dopants would find themselves confined to one-dimensional lines. In this situation, their interactions generically induce non-Fermi liquid behavior, including spin-charge separation. Also, the walls must be treated as dynamical objects – for example, even if a long wall is pinned by impurities at several locations it will be able to wiggle in between, and there will be an effective “electron-phonon” interaction of quite unusual type between its wiggles and the dopants. It may be that such dynamics is rich and peculiar enough to accommodate the cuprates, or some of the other bad actors in solid state physics.

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