Nagaoka problem and RVB: an unexpected connection

A resonant valence bond spin liquid in the dilute limit of doped frustrated Mott insulators
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Recommended with a Commentary by Frédéric Mila, Ecole Polytechnique Fédérale de Lausanne, Switzerland

When a quantum particle moves on a Bravais lattice, its dispersion is just the sum of the Fourier transforms of the hopping integrals. For a square lattice with nearest-neighbour hopping $-t$, it is simply given by

$$\epsilon_{\text{square}}(\vec{k}) = -2t(\cos k_x + \cos k_y).$$

If one adds a diagonal coupling in one direction to mimic the topology of the triangular lattice, it becomes

$$\epsilon_{\text{triangular}}(\vec{k}) = -2t(\cos k_x + \cos k_y + \cos(k_x + k_y)).$$

The dispersions are represented in Fig.1 for both signs of t. For the square lattice, the minimum energy is given by $-4|t|$ for both signs of t. For the triangular lattice however, it depends on the sign of t. It is equal to $-6|t|$ if $t > 0$ (negative hopping integral with the standard convention), but only to $-2|t|$ if $t < 0$ (positive hopping integral).

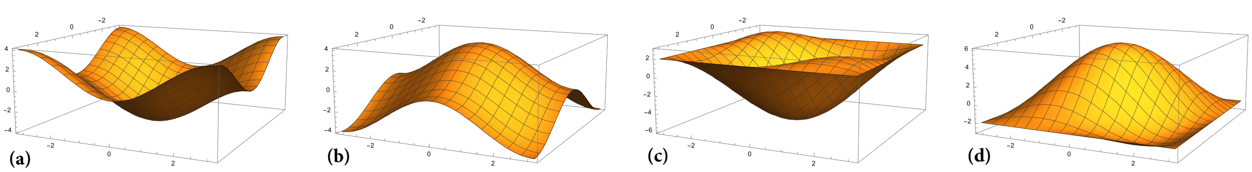

Figure 1: Dispersion of a particle on the square and triangular lattice (square lattice with one diagonal). (a) Square lattice with $t > 0$; (b) Square lattice with $t < 0$; (c) Triangular lattice with $t > 0$; (d) Triangular lattice with $t < 0$.

Now let us suppose that the particle moves on a lattice where at each site there is a spin-1/2, a problem known as the Nagaoka problem. On a lattice of N sites the Hilbert space is now of dimension $N \times 2^{N-1}$, where the factor N comes from the position of the particle and the factor 2^{N-1} from the $(N-1)$ spins-1/2. What is the ground state energy? The solution depends crucially on the lattice and on the sign of t.

For a Bravais lattice with nearest-neighbor hopping, it is easy to show that the energy cannot be lower than $-z|t|$, where z is the coordination of the lattice. If one assumes that all spins are parallel (i.e. if one works in sector $S^z_{\text{total}} = (N-1)/2$), the dispersion is the same as that of a particle alone. For the square lattice, this implies that this lower bound is reached in that sector. This is the essence of the *Nagaoka effect*[1]: A hole in the Hubbard model with U infinite (hence with no exchange between the spins) induces ferromagnetic order.

For the triangular lattice however, this is only true if $t > 0$. If $t < 0$, the lowest energy one can reach in this sector is only $-2|t|$, very far from the lower bound $-6|t|$. Can one do better in other sectors? This question has been addressed by Haerter and Shastry in 2005[2], who have shown that one can indeed do much better. In the sector $S^z_{\text{total}} = 0$, the ground state energy is slightly below $-4|t|$ on 21 and 27 sites clusters. Furthermore the ground state exhibits a 3-sublattice structure typical of antiferromagnetic coupling between the spins, hence the conclusion that holes induce antiferromagnetic order in that case, and the prediction that the antiferromagnetic coupling is proportional to the doping. This is sometimes called the *counter-Nagaoka* effect. Note that the true ground state wave-function is no longer simple to write down, and the energy is not a simple number.

Haerter and Shastry identified the essence of the problem as the presence of odd loops with a positive hopping integral. One can thus expect that a similar problem will show up on any lattice with odd loops, and for one type of charge carrier, a hole or a doubly occupied site, since the sign of the hopping changes in a particle-hole transformation.

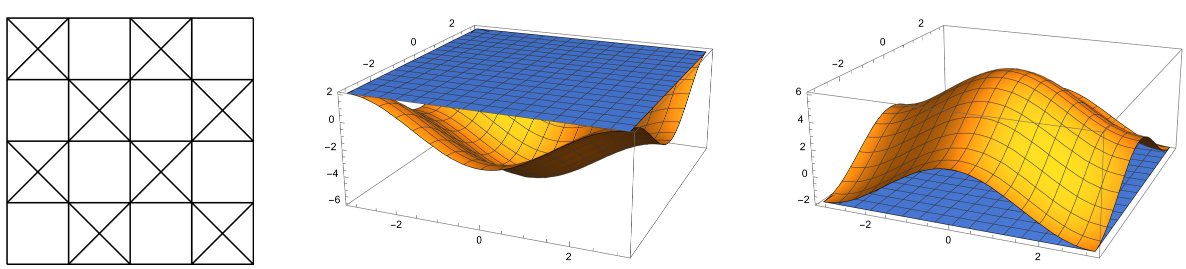

Figure 2: Left: Checkerboard lattice; Middle: Dispersion on the checkerboard lattice with $t > 0$; Right: Dispersion on the checkerboard lattice with $t < 0$.

The first hint that in some cases there might be a simple analytical solution even for $t < 0$ (positive hopping) can actually be found in the numerical results obtained on the checkerboard lattice (Fig.2) by Poilblanc one year earlier[3]. For that lattice, there are two sites per unit cell, hence two branches. Their dispersion is given by

$$\epsilon^{(+)}_{\text{checkerboard}}(\vec{k}) = -2t(1 + \cos k_x + \cos k_y), \quad \epsilon^{(-)}_{\text{checkerboard}}(\vec{k}) = 2t,$$

where the directions x and y are along the diagonals (see Figs. 2). While, for $t < 0$, the minimal energy of the ferromagnetic state is $-2|t|$, he found that the ground state energy is $-4|t|$ for one hole and $-8|t|$ for two holes on small clusters, in a state which is of course not at all ferromagnetic. The magnetic background manages to suppress the quantum interferences that are responsible for the loss of kinetic energy in the ferromagnetic state in such a way that the energy is still a simple number. An exact solution has actually been obtained on the Husimi cactus by Kim[4], who showed that on this tree-like lattice a hole moves in a valence-bond pattern.

The implications of these results regarding the nature of the magnetic state promoted by the hole motion with $t < 0$ in the checkerboard lattice have been overlooked however until Glittum et al addressed the question on the pyrochlore lattice[5], a 3D lattice of corner sharing tetrahedra (of which the checkerboard lattice is a 2D version) and showed analytically (i) that there is a lower bound of $-4|t|$, and (ii) that this lower bound can be saturated by a wave-function that they could write down explicitly. And quite remarkably, this wave-function is a superposition of states with one hole and all dimer coverings of the pyrochlore lattice with one dimer per tetrahedron. The conclusion is thus that holes moving on a lattice with corner sharing tetrahedra induce a resonating valence bond (RVB) state, the type of ground state postulated by Anderson and Fazekas for the triangular lattice in the seventies[6, 7].

What are the physical implications of this exact result? The first question that comes to mind is whether this mechanism can be related to superconductivity, following up on Anderson's RVB theory of superconductivity of the high T_c cuprates[9]. As the authors admit however, this is unclear at that stage.

The second less ambitious but nevertheless very important question is whether this effect is limited to infinite U because this would considerably limit the impact of this result. It sounds like one can be reasonably confident that the effect will persist for finite U for several reasons. First of all, a finite U tends to induce antiferromagnetic interactions between the spins. For the Nagaoka effect this is of course a big problem because these interactions directly compete with ferromagnetic order. But here, since the wave-function that allows the hole to gain kinetic energy is built with nearest-neighbour singlets, lowering U might actually cooperate. The possibility to realize an RVB ground state even at half-filling due to finite U and super-exchange has actually been suggested by Normand and Nussinov[8], who realized that to third order in t/U, and for $t/U = 1/\sqrt{30}$, the effective model is a sum of projectors on spin-2 on each tetrahedron, so that any wave function with at least one dimer singlet per tetrahedron is a ground state. So maybe there is indeed an RVB phase extending to not too large U and to not too small doping on the pyrochlore lattice, and by extension on lattices of corner sharing tetrahedra such as the checkerboard lattice.

Finally, this raises yet another interesting question: What about other lattices with odd loops? Which kinds of states can be stabilized by holes moving with a positive hopping amplitude? Considering the wealth of exotic quantum phases discussed in frustrated magnets, there is potentially room for interesting discoveries in the investigation of the Nagaoka effect on other frustrated geometries.

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