Cooper instability of a metallic phase in the Hubbard model with repulsion

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The Hubbard model with a local repulsion and a half-filled band is analyzed on a hypercubic lattice. A canonical transformation to electrons and holes reveals a local attraction of these entities and a Cooper instability with respect to their combining to form neutral pairs, i.e., excitons. The ground state of the model is thus an insulator for any finite interaction. It is a state like that of the BCS model, in which excitons play the role of the Cooper pairs.

The Hubbard Hamiltonian

$$H=-t\sum_{\langle \mathbf{nl}\rangle}(c^+_{\mathbf{n}\uparrow}c_{\mathbf{l}\uparrow}+c^+_{\mathbf{n}\downarrow}c_{\mathbf{l}\downarrow})+U\sum_{\mathbf{m}}c^+_{\mathbf{m}\uparrow}c_{\mathbf{m}\uparrow}c^+_{\mathbf{m}\downarrow}c_{\mathbf{m}\downarrow} \tag{1}$$

with a local repulsion, $U>0$, and a half-filled band,

$$\sum_{\mathbf{m}}(c^+_{\mathbf{m}\uparrow}c_{\mathbf{m}\uparrow}+c^+_{\mathbf{m}\downarrow}c_{\mathbf{m}\downarrow})=N, \tag{2}$$

has been proposed[1] as the simplest electronic model of the metal–insulator transition (N is the total number of sites). According to Hubbard's intention and widespread opinion, this model should describe both a metallic state with sufficiently small U and a transition to an insulating phase at some U_c.

The transition theory proposed by Hubbard[2] did indeed lead to a finite U_c. However, that theory is recognized as suffering from several serious shortcomings.[3] The most obvious one is the paramagnetism of the insulating phase.

In the present letter we show that the model of (1), (2) reduces to the BCS model, which has been studied thoroughly, so the former model can thus be studied by the methods of superconductivity theory. Such a study shows that a metal–insulator transition does not occur at absolute zero in the Hubbard model.

Let us examine model (1), (2) on a unit lattice, which will be cubic, quadratic, or linear, depending on the dimensionality. We introduce new Fermi operators through the canonical transformation[4]

$$h_{\mathbf{m}}=e^{i\mathbf{qm}}c^+_{\mathbf{m}\uparrow},\quad h^+_{\mathbf{m}}=e^{-i\mathbf{qm}}c_{\mathbf{m}\uparrow},$$
$$e_{\mathbf{m}}=c_{\mathbf{m}\downarrow},\quad e^+_{\mathbf{m}}=c^+_{\mathbf{m}\downarrow}, \tag{3}$$

where the components of the wave vector satisfy $q_\alpha=\pi$. It is easy to verify that $|\mathbf{vac}\rangle$, i.e., the vacuum of $e_{\mathbf{m}}$ and $h_{\mathbf{m}}$ fermions,

$$e_{\mathbf{m}}|\mathbf{vac}\rangle=0, \quad h_{\mathbf{m}}|\mathbf{vac}\rangle=0 \tag{4}$$

is the singly filled state

$$|\mathbf{vac}\rangle=\prod_{\mathbf{m}} c^{+}_{\mathbf{m}\uparrow}|0\rangle. \tag{5}$$

The operators $e^{+}_{\mathbf{m}}$ and $h^{+}_{\mathbf{m}}$ create an extra electron and an extra hole, respectively:

$$e^{+}_{\mathbf{m}}|\mathbf{vac}\rangle=c^{+}_{\mathbf{m}\downarrow}\prod_{\mathbf{n}} c^{+}_{\mathbf{n}\uparrow}|0\rangle,$$

$$h^{+}_{\mathbf{m}}|\mathbf{vac}\rangle=e^{i\mathbf{q}\mathbf{m}}c_{\mathbf{m}\uparrow}\prod_{\mathbf{n}} c^{+}_{\mathbf{n}\uparrow}|0\rangle. \tag{6}$$

In terms of the operators $h_{\mathbf{m}}$ and $e_{\mathbf{m}}$, Hamiltonian (1) and condition (2) become

$$H=-t\sum_{\langle\mathbf{nl}\rangle}(h^{+}_{\mathbf{n}}h_{\mathbf{l}}+e^{+}_{\mathbf{n}}e_{\mathbf{l}})-U\sum_{\mathbf{m}}h^{+}_{\mathbf{m}}h_{\mathbf{m}}e^{+}_{\mathbf{m}}e_{\mathbf{m}}+\frac{U}{2}\sum_{\mathbf{m}}(h^{+}_{\mathbf{m}}h_{\mathbf{m}}+e^{+}_{\mathbf{m}}e_{\mathbf{m}}) \tag{7}$$

$$\sum_{\mathbf{m}}(h^{+}_{\mathbf{m}}h_{\mathbf{m}}-e^{+}_{\mathbf{m}}e_{\mathbf{m}})=0. \tag{8}$$

When we go over to the momentum representation, expression (7) takes the form of the BCS Hamiltonian:[5]

$$H=\sum_{\mathbf{k}}\epsilon_{\mathbf{k}}(h^{+}_{\mathbf{k}}h_{\mathbf{k}}+e^{+}_{\mathbf{k}}e_{\mathbf{k}})-\frac{U}{N}\sum_{\mathbf{pgk}}h^{+}_{\mathbf{p}+\mathbf{k}}h_{\mathbf{p}}e^{+}_{\mathbf{g}-\mathbf{k}}e_{\mathbf{g}}, \tag{9}$$

which describes a system of attractive fermions with a seed spectrum

$$\epsilon_{\mathbf{k}}=\frac{U}{2}-t_{\mathbf{k}}, \quad t_{\mathbf{k}}=2t\sum_{\alpha}\cos k_{\alpha}. \tag{10}$$

We are interested primarily in the region of small values of U, where we might expect a metallic behavior. We know[5,6] that this region, $U/t\ll 1$, is described exceptionally well by the BCS variational wave function which underlies superconductivity theory:

$$|\psi\rangle=\prod_{\mathbf{k}}(u_{\mathbf{k}}+v_{\mathbf{k}}e^{+}_{\mathbf{k}}h^{+}_{-\mathbf{k}})|\mathbf{vac}\rangle. \tag{11}$$

Condition (8), which is actually the condition for a half-filled band, is satisfied automatically.

A calculation in BCS theory quickly gives us the spectrum of excitations

$$E_{\mathbf{k}}=(4t^2_{\mathbf{k}}+\Delta^2)^{1/2}, \tag{12}$$

where the gap Δ can be found from the equation

$$\sum_{\mathbf{k}}(4t^2_{\mathbf{k}}+\Delta^2)^{-1/2}=\frac{N}{U}. \tag{13}$$

Solving this equation, we find several gap sizes, depending on the dimensionality D:

$$\Delta \approx \begin{cases} 16t\exp - 2\pi t/U & (1D), \\ 64t\exp - 2\pi\sqrt{t/U} & (2D), \\ 24t\exp - 7.06t/U & (3D). \end{cases} \tag{14}$$

We also find an antiferromagnetic order:

$$\langle S^z_{\mathbf{m}} \rangle = 0, \quad \langle S^+_{\mathbf{m}} \rangle = \langle c^+_{\mathbf{m}\uparrow} c_{\mathbf{m}\downarrow} \rangle = (\Delta/2U) e^{-i\mathbf{qm}}. \tag{15}$$

The amplitude of the local spin density, $\Delta/2U$, vanishes in the limit $U \to 0$.

The existence of a nonvanishing gap in spectrum (12) means that the ground state of the Hubbard model is insulating for any finite U. This behavior agrees entirely with the exact one-dimensional solution of Lieb and Wu.[7] The exact transformation of Hamiltonian (1) into (9) essentially means that the ground state of the Hubbard model with a half-filled band is an insulating state to the extent that the ground state of the BCS model is a superconducting state. In other words, we wish to stress that the variational approximation adopted above is as reliable as the BCS model in superconductivity theory.

A transition to an insulating state should be interpreted as the binding of electrons and holes to form neutral excitons, which constitute analogs of Cooper pairs. Like the Cooper instability in superconductivity theory, the transition to the insulating phase in the Hubbard model occurs for an arbitrarily weak interaction.

It is also obvious that the half-filling is critically important for the formation of the insulating phase. When there is a deviation from half-filling, conditions (2) and thus (8) are violated; i.e., the numbers of electrons and holes become different. Free charged carriers thus appear along with the neutral excitons in the ground state, so the system becomes metallic.

Drawing further on this analogy with superconductivity, we can also assert that the gap vanishes at a temperature $T_c \sim \Delta$. The antiferromagnetic insulator undergoes a second-order phase transition to a paramagnetic metal.

Our conclusion that a transition does not occur applies only to the Hubbard model on lattices of a certain (although extremely broad) class. Specifically, the transformation to the BCS model in (3) is possible only under the following condition: There must exist a vector $\mathbf{q}$ which satisfies the condition $\mathbf{q}\vec{\delta} = \pi$ for any elementary translation $\vec{\delta}$. This condition is satisfied on "bipartite"[8] lattices. A bipartite lattice is one which we can, in our imagination, split in two in such a way that all the nearest neighbors of any site of the first sublattice belong to the second sublattice, and vice versa. Cubic, quadratic, and linear lattices are bipartite lattices.

In summary, we can assert that the metallic phase and the metal–insulator transition at absolute zero do not exist in the Hubbard model on a bipartite lattice. It should be noted in this connection that a phase transition has been observed[8] on a triangular lattice, which is not bipartite.

Anticipating a possible criticism, we would like to stress the following point: There is indeed a difference between BCS theory and the Hubbard case. In the BCS theory, only those electrons which are in a Debye neighborhood of the Fermi surface are attracted to each other, while in Hamiltonian (9) this attraction occurs throughout the Brillouin zone. However, this difference would only strengthen the tendency toward pairing and thus toward a transition to an insulating state.

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