The Mott transition and superconductivity

G. M. Éliashberg
L. D. Landau Institute of Theoretical Physics, Russian Academy of Sciences, 142432 Chernogolovka, Moscow Region, Russia

W. von der Linden
Physics Institute, Würzburg University, 97074 Würzburg, Germany

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If a Mott transition is not accompanied by changes in the crystal symmetry or the magnetic symmetry, a state with a split conduction band would have to be a phase-coherent state, to which the Luttinger theorem does not apply. From this standpoint, a superconducting state is a realization of a Mott state. Numerical data for the 1D Hubbard model illustrate this conclusion.

Despite the voluminous literature on the Mott transition, the nature of a state with a split conduction band[1] remains a matter of debate. In this letter we wish to discuss a relationship between this state and a superconductor, using as an analysis tool the sum rule of Luttinger and Ward (also known as the "Luttinger theorem").[2,3] The general conclusions reached below are illustrated by numerical data for the 1D Hubbard model, in which the Mott state is realized in the case of a half-filled band.[4] Our calculations differ from other cluster calculations of this model (e.g., Refs. 5 and 6) in the particular choice of the quantities to be calculated. One of these quantities is a spectrum in terms of which the Luttinger theorem is formulated. Being an exact relation for the number of particles, this theorem does not hold in superfluid Fermi systems, in which the number of particles fluctuates in the ground state at a given value of the chemical potential (or of the electrochemical potential, for electrons), because of macroscopic phase coherence.[7] The Luttinger theorem is thus a characteristic property of "normal systems," and only for such systems can a corresponding one-particle spectrum be determined. For noninteracting particles (and in the Hartree–Fock approximation), this spectrum is the same as the ordinary spectrum, but (in contrast with a spectrum of excitations) it remains strictly defined even when there are correlation effects. Correlation effects are particularly important in crystals with strongly coupled electrons, and this spectrum is the only well-defined band spectrum in this situation. For this reason this spectrum should become the target of microscopic band-theory calculations for correlated systems. We hope that our calculations for a very simple model will demonstrate the usefullness of this approach.

We begin by reproducing some general relations,[9] using the following definition of the Green's function:

$$\hat{G}_R(\epsilon)=i\int_0^\infty e^{i\epsilon t}\hat{A}(t)dt, \quad \hat{G}_A(\epsilon)=-i\int_{-\infty}^0 e^{i\epsilon t}\hat{A}(t)dt, \tag{1}$$

$$\hat{A}(t)\equiv A(t;x,x')=\langle\{\psi(t,x),\psi^+(0,x')\}\rangle,$$

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where ψ^+ and ψ are particle creation and annihilation operators in the Heisenberg picture with an evolution operator $\exp[-i(H-\mu N)t]$; x, x' incorporate the spatial coordinates r, r' and the spin coordinates σ, σ'; and $\langle \dots \rangle$ means a thermodynamic average over a grand canonical ensemble. The chemical potential μ is determined as a function of the temperature for a given number of particles N in the volume V from the general expression for the number of particles:

$$N=\int_{-\infty}^{0} \frac{1}{e^{\epsilon/T}+1} \operatorname{Tr} \hat{\rho}(\epsilon) d\epsilon. \tag{2}$$

The spectral-density operator

$$\hat{\rho}(\epsilon)=\frac{1}{2\pi i}[\hat{G}_R(\epsilon)-\hat{G}_A(\epsilon)] \tag{3}$$

satisfies the integral condition

$$\int_{-\infty}^{\infty} \hat{\rho}(\epsilon) d\epsilon=\delta(r-r')\delta_{\sigma\sigma'}, \tag{4}$$

which follows immediately from definition (1).

We can now formulate the Luttinger theorem, which is often understood as a proof of Landau's postulate that the Fermi momentum is independent of the interaction[8] and its generalization to electrons in a metal. This theorem actually contains two assertions.

1. For a certain class of Fermi systems, the anti-Hermitian part of the operator $\hat{G}_R^{-1}(\epsilon)$ in the ground state vanishes at $\epsilon=0$. There thus exists a one-particle spectrum (for brevity, a "ξ-spectrum") which is determined by the Hermitian operator $\hat{\xi}$:

$$\hat{G}_R^{-1}(0)=\hat{G}_A^{-1}(0)=\xi. \tag{5}$$

2. The number of negative eigenvalues ($\xi_\alpha<0$) of the operator $\hat{\xi}$ is equal to the number of particles, N, if the chemical potential is found from Eq. (2) at $T=0$:

$$N=\sum_{\xi_\alpha<0} 1. \tag{6}$$

The derivation of this theorem which was carried out for an isotropic system[2] (a Fermi liquid) and then repeated, without substantial changes, for electrons in a nonmagnetic crystal[3] is actually not limited by any assumptions regarding the crystal symmetry or magnetic symmetry of the ground state: In each case, a one-electron "Hamiltonian" $\hat{\xi}$ which has the corresponding symmetry can be determined, and its spectrum satisfies sum rule (6). For electrons in an ideal crystal, the operator $\hat{\xi}$ is diagonal in the Bloch spinor representation $\varphi_{n,k}(x)$ ($x=r,\sigma$; n is a band index; and k is the wave vector in the Brillouin zone). In the absence of magnetism, or in the case of a simple antiferromagnetic order, the bands are doubly degenerate, and we can single out the index $\nu=1, 2$. Below we will be thinking of specifically these cases, since they are pertinent to the problem stated in the title of this letter.

Much of band-theory phenomenology remains in force in terms of the ξ-spectrum. In particular, we can, as in the approximation of a self-consistent field, distinguish between metals and insulators on the basis of the filling of bands. By virtue of the Luttinger theorem, this filling of bands is related to the electron stoichiometry. It is important to stress here that in the case of a metal the ξ-spectrum determines not only the Fermi surface, $\xi_{nkv}=0$, but also the density of states of electrons at this surface: It follows from Eqs. (3) and (5) that we have $\langle\alpha|\hat{\rho}(0)|\alpha\rangle=\delta(\xi_\alpha)$, and the total density of states on S_F is

$$\rho_F=V\cdot 2\int\frac{dS_F}{|v|}, \tag{7}$$

where $v=d\xi_k/dk_\perp$ is the derivative along the normal to S_F. The quantity ρ_F is the density of states which is tested in experiments involving the removal of an electron from a metal or the injection of an electron into a metal. This parameter is not part of the Fermi-liquid phenomenology. It is always smaller than the density of states of quasiparticles (or excitations). These two quantities are the same only in the Hartree–Fock approximation (see Ref. 9 for more details regarding the relationship with Fermi-liquid theory).

When Mott advanced his famous hypothesis, it immediately became clear that a state with a split conduction band in a crystal with an odd number of electrons per unit cell was a consequence of correlation effects and was incompatible with a band theory based on the approximation of a self-consistent field. Now we see that the same considerations make it incompatible with the existence of a ξ-spectrum. Nor do correlated normal systems, which are controlled by the Luttinger theorem, have any place for this state. As has been pointed out elsewhere,[7,9] a superconductor is an anomalous system (and so far the only one among the known electronic systems), about which it can be said that the Luttinger theorem definitely does not work. In this sense a superconducting state is a realization of a Mott state.

An instructive illustration of the approach described above is a calculation of the ξ-spectrum for the 1D Hubbard model. A calculation was carried out for a cluster of ten sites on a ring, and an exact diagonalization was carried out by a method approximately the same as that which has been used by other authors.[5,6] These calculations were carried out for various numbers of particles $N\leqslant 10$ and for the values $U=1$, 4, 8, and 16 (in units of t). To save space in this letter, we present only some of the results in Figs. 1 and 2. Before we discuss these results, we would like to point out some important properties of the model. As in any single-band model, the operator $\hat{G}(\epsilon)$ is diagonal in the k representation, and from definitions (1) and (3) we have

$$G_R(\epsilon,k)=\int_{-\infty}^{\infty}\frac{\rho_k(E)}{E-\epsilon-i\delta}\,dE. \tag{8}$$

For a half-filled band the total spectral density $\rho(E)$ has a gap, which is symmetric with respect to $E=0$ ($\mu_+-\mu_-$ in the notation of Lieb and Wu[4]). At $U\ll t$, this gap is exponentially small. From the definition of ξ_k we have

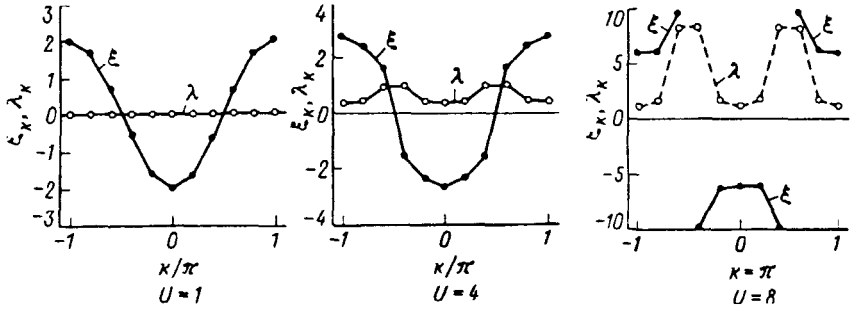

FIG. 1.

$$\frac{1}{\xi_k}=\int_{-\infty}^{\infty}\frac{\rho_k(E)}{E}\,dE, \tag{9}$$

and by virtue of the known particle–hole symmetry we have

$$\rho_k(E)=\rho_{\pi-k}(-E), \quad \xi_K=-\xi_{\pi-k}. \tag{10}$$

It is not difficult to see that ξ_k changes sign at $|k|=k_F=\pi/2$ (the length of the cell is $a=1$), but does not pass through zero: There is also a gap in the ξ_k spectrum. Two cases, corresponding to completely different physical situations, are possible here.

1. The discontinuity in ξ_k at $|k|=\pi/2$ is of finite magnitude. In this case we have an ordinary insulator, and the spectrum may lead to a Brillouin zone smaller by a factor of 2. Such a state might be called a "marginal antiferromagnet."

2. The partial density $\rho_k(E)$ varies continuously as the Fermi boundary is crossed, and in this case we have $G(0,k_F)=0$. The ξ spectrum thus diverges. The Luttinger theorem does not hold in this state in the macroscopic limit; i.e., we are dealing with a marginal superconductor. By way of comparison, here is the expression for $G_R^{-1}(0,k)$ in the single-band BCS model, which follows directly from the paper by Gor'kov:[10]

$$G_R^{-1}(0,k)=v(k-k_F)+\frac{\Delta^2}{v(k-k_F)+i\delta}. \tag{11}$$

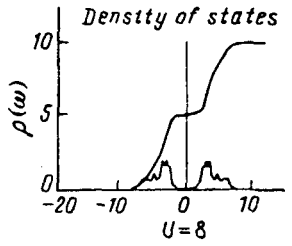

FIG. 2.

We see that in this case there is again a dramatic transformation of the ξ-spectrum, and condition (5) does not hold.

The results in Fig. 1 do not support a definite choice of one of these two situations, although at $U=8$ we do see a tendency for a divergence of the spectrum. This divergence is also indicated by the anomalously strong dispersion $\lambda(k)$, which is given by

$$1+\lambda(k)=-\frac{\partial}{\partial\epsilon}\left[G_R^{-1}(\epsilon,k)\right]_{\epsilon=0}.$$

The physical meaning of this quantity has been discussed in detail previously.[7,9] It should of course be possible to find an unambiguous answer to the question from the exact solution of Lieb and Wu; that would be an extremely interesting problem. Figure 2 shows the total spectral density for $U=8$; it has the shape typical of a Mott state. The second curve here—the integral of the spectral density—is used to monitor the satisfaction of completeness condition (4). These results, as well as other results on the spectral density, not shown here, agree with calculations by Meinders *et al.*[5]

In conclusion we wish to stress that the analysis carried out in this letter not only reveals a new aspect of the Mott-transition problem, but also shows that a formulation of superconductivity theory, which is more general than the BCS theory, does not have to be based on an initially normal metallic state: Band theory does not apply to a superconductor, even in terms of the ξ-spectrum, and the corresponding formalism does not have to "remember" such concepts as a Fermi surface and the density of states on it.

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