Singular Forward Scattering in the 2D Hubbard Model and a Renormalized Bethe Ansatz Ground State

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(Received 23 July 1990)

In a recent Letter we argued that the existence of an upper Hubbard band necessarily would lead to Luttinger liquid ($Z=0$) properties for a strongly interacting electron gas, as opposed to Fermi liquid. In this paper we identify the singular scattering diagrams and make a hypothesis about the form of the ground state of the 2D Hubbard model.

PACS numbers: 75.10.Lp, 74.65.+n, 74.70.Vg

In a recent Letter[1] we argued that the existence of an upper Hubbard band necessarily would lead to Luttinger liquid ($Z=0$) properties for a strongly interacting electron gas, as opposed to Fermi liquid. In this paper we identify the singular scattering diagrams and make a hypothesis about the form of the ground state of the 2D Hubbard model.

In order to demonstrate the singularity, we assume that the state is a Fermi liquid and show that forward scattering modifies the state in a singular way. The most extensively studied 2D problem is the low-density limit, studied by Galitskii[2] and Bloom,[3] and known by expansion in n to go to a Fermi-liquid limit as $n\rightarrow 0$. We do not quarrel with this but identify new singular terms proportional to $(\ln n)^{-1}$ which are controlling for all finite n. The relevant terms must be treated outside conventional many-body perturbation theory because they enter not in the standard perturbation series as conventionally used but in the initial determination of the scattering vertex or "pseudopotential" to be used in that theory, i.e., in replacing the bare scattering potential V by a "scattering matrix" T which describes the local response of the wave function of one particle to the potential of another. Unfortunately, T has very complex low-energy singularities on the "energy shell" which depend crucially on boundary conditions, and once boundary conditions are included forward and backward scattering are no longer clearly distinguishable. The correct treatment of the singularity can always be managed by directly calculating the energy shift in the particle-particle channel, which we now do.

Schrödinger's equation for an eigenstate with energy E of the two-particle scattering problem in a channel of momentum $2k$ for a pair of opposite-spin particles reduces to[4]

$$L^D/U=\sum_Q(E-\epsilon_{k+Q}-\epsilon_{k-Q})^{-1}. \qquad (1)$$

Let $\epsilon_{k+Q}+\epsilon_{k-Q}=E_Q$, where $2Q$ is the relative momentum of the particles in a given intermediate state. There will be an eigenvalue E of (1) above every value of E_Q and below the next one; the lowest one, $E(Q=0)$, will be that for forward scattering, and we may write $[E(Q=0)-E_0]/(E_1-E_0)=\delta/\pi$, where δ is the phase shift in the isotropic channel. (We use the low-density limit to justify the simplifying assumption that the problem is approximately Galilean for small Q. The higher energies E_Q will not satisfy this, but they only enter in upper limits of integrals. The arguments go through, but less simply, for any k.) The sum in (1) diverges at low Q in 1D, and as a result in 1D, $\delta=\pi$ independently of U and of the upper limit. This means that at low density opposite spins effectively obey an exclusion principle in 1D as is well known from the Hubbard model literature. In 3D the sum converges at the low end, and is controlled by the large values of Q, so that in general even for large U

$$1/(E-E_0)\sim L^3,$$

and since E_1-E_0 is $\sim L^2$, $\delta\rightarrow 0$ as $1/L$; this is conventional scattering length theory and leads to the Fermi liquid. However, in this case the $l=0$ channel must be treated more carefully, which we have not yet done. In 2D, the sum diverges at both ends logarithmically, and the eigenvalue equation reduces to

$$\frac{1}{E-E_0}-L^2P\int_{\pi/L}^{\pi/a}\frac{d^2Q}{E_Q-E}=\frac{L^2}{U},$$

$$\frac{1}{E-E_0}\simeq L^2\ln\frac{1}{a^2Q_{\min}^2},$$

so that $\delta\sim 1/\ln L$ which, as Bloom showed, represents a divergent scattering length but is sufficiently small to allow a Fermi-liquid theory. Note the relevance of the upper cutoff π/a; the problems do not occur for free particles, with $a\rightarrow 0$.

Something quite new happens if we go to finite (if small) density and consider particle-particle scattering at the Fermi momentum k_F ($k=2k_F$). Now we must exclude occupied states from the sum in (1) and it reads

$$\frac{L^2}{U}=\sum_Q{}'\frac{1}{E-E_Q}, \qquad (2)$$

where $\sum'$ implies that neither $k+Q$ nor $k-Q$ is inside the Fermi surface. Figure 1 shows the effect of this ex-

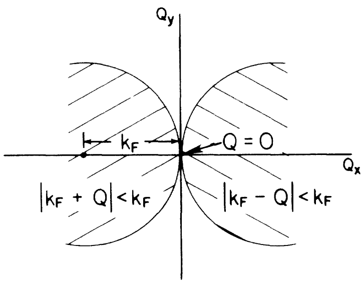

FIG. 1. Region of recoil momentum Q excluded by the Pauli principle.

clusion: It removes all but a fraction $Q^2/\pi k_F^2$ of the phase space at a given small $|Q|$. This eliminates the "recoil" effect which we might expect would prevent singularities. Now the principal part integral converges nicely, behaving like $(1/k_F^2)\int Q^2 Q\,dQ/(E_Q - E_0)$ for small Q. For small k_F the singular term becomes $\ln(1/k_F^2 a^2)$. Therefore the phase shift becomes finite, of order $\delta \sim \pi/2\ln(k_F a)$. As k_F increases, we have in general a finite phase shift δ somewhere between 0 and π. A finite phase shift for forward scattering has very severe consequences for Fermi-liquid theory. In particular, it means that two particles (or quasiparticles) of opposite spin may *not* occupy the same plane-wave state, as is assumed in Landau theory, in which it is assumed the fixed point is the free Fermi gas. It also implies that the renormalization constant

$$Z \sim e^{-(\delta/\pi)^2 \ln L^2} \to 0\,. \tag{3}$$

Recognizing that for finite time or frequency, $(L^2)_{\rm eff} \sim v_F^2/\omega^2$, this gives us a form for the singularity,

$$Z(\omega) \sim -\left(\frac{\partial\Sigma}{\partial\omega}\right)^{-1} \sim \omega^{(\delta/\pi)^2}\,; \tag{4}$$

for small δ, this closely resembles the $\ln\omega$ behavior proposed on experimental grounds.[5]

Finally, we note that the only way an effective intraparticle potential can lead to a finite phase shift for forward scattering is for it to be long ranged. Thus we could model the effect of the exclusion principle on forward scattering as a long-range pseudopotential $\sim 1/r$, which is the major effect of the gauge field proposed as another way of enforcing the projective transformation eliminating the "upper Hubbard band." This approach is thus not necessarily in conflict with gauge theory methods.

We should reiterate that Landau's Fermi-liquid theory is based on the consideration of relative energy scales, equivalent to a renormalization-group theory. The relevant, fixed-point Hamiltonian $\mathcal{H}^*$ is the free Fermi gas; the Landau interactions $f_{kk'}n_k n_{k'}$, which embody only the renormalized Hartree forward and backward scattering terms, are marginal, i.e., of order ω or T, and all of many-body perturbation theory is irrelevant at the fixed point, i.e., of order ω^2 or T^2, which makes it hard to pick up the difficulties in that theory. Haldane's "Luttinger-liquid" theory,[6] which is the one-dimensional response to diverging Hartree terms, rediagonalizes the first two terms in the hope that scattering will still be irrelevant, since one has done as little damage to Fermi-liquid theory as possible. We now try to carry out the same program in 2D, but of course, unlike the above, we must now move into speculative territory.

To do this we follow Fermi-liquid theory in doing first a conventional renormalization eliminating high-energy virtual scatterings, and assume that the remaining "quasiparticle" states involved in low-energy excitations all have momenta near a Fermi surface. This elimination will only have made the effective singular forward scattering bigger.

At this point we are talking about renormalized, "quasiparticle" states, which have singular density-density interactions but all virtual scatterings into high-momentum states are renormalized away. Whether Fermi liquid or not, simple geometry shows that all real scatterings of pairs of particles near a Fermi surface are "nondiffractive" in Sutherland's sense: The momenta are conserved, only spin can be exchanged. Thus for the effective particles, a Bethe ansatz may be assumed:

$$\Psi = \sum_{P,Q} \exp\left(\sum k_{Q_i} x_{P_j}\right)[Q,P]\,,$$

with the set of k's invariant. The $[Q,P]$ determine the spin state; the k's determine how charge moves. But the effect of singular forward scattering is to tell us that the set of k's occupy a volume in k space greater than that of the Luttinger Fermi surface; this is precisely what happens in the one-dimensional case. In this event the distribution of k's has *no singularity* near the Fermi surface and all low-energy charge motion takes place by collective "sliding" motions of the k distribution. (As in 1D, the k's are not real particle momenta and do not determine the Fermi surface which depends on the spin motions alone.) Following Luther,[7] we can rewrite the free-particle Hamiltonian in terms of charge- and spin-density waves moving in a given direction Ω with Fermi velocity v_F. The spin-density waves encounter no singular scattering (triplet pairs do not forward scatter) but the charge-density waves must be rediagonalized by the standard Bogoliubov transformation to take into account the singular scattering, thus leading to different charge and spin velocities and to charge-spin separation. The collective charge modes may be thought of as "holons" but are not particlelike. In particular, they are not affected by elastic scattering, by an argument similar to the "dirty superconductor" theorem.[8] Residual resistance can be caused only by spin scattering. We suggest that the state may be considered to be a $T_c = 0$ superconductor, in the absence of spin scattering. More detailed discussion of specific properties will be published elsewhere.[9]

I acknowledge stimulating discussions with S. Sorella, E. Lieb, and constant input from Y. Ren. This work was supported in part by the National Science Foundation, Grant No. DMR-8518163, and by the U.S. Department of the Air Force, Grant No. AFOSR 87-0392.

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