

“Luttinger-Liquid” Behavior of the Normal Metallic State of the 2D Hubbard Model

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Analysis of interacting fermion systems shows that there are two fundamentally different fixed points, Fermi-liquid theory and “Luttinger-liquid theory” (Haldane), a state in which charge and spin acquire distinct spectra and correlations have unusual exponents. The Luttinger liquids include most interacting one-dimensional systems, and some higher- (especially two) dimensional systems in which the band spectrum is bounded above: systems with Mott-Hubbard gaps and an upper Hubbard band. We give a theory which is useful in calculating normal-state, and some superconducting, properties of high- T_c superconductors.

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Haldane¹ has characterized the behavior of a large variety of one-dimensional quantum fluids by the term “Luttinger liquid,” showing that they can all be solved by common techniques based on transforming to phase and phase-shift variables for the Fermi-surface excitations (a procedure often called “bosonization” even though some of the Luttinger liquids start out as Bose systems). These systems are characterized by fractionation of quantum numbers—e.g., in the Heisenberg spin chain the excitations are spin- $\frac{1}{2}$ fermionlike, while in the Hubbard model they are spin- $\frac{1}{2}$ chargeless spinons and $\pm e$ spinless holons with fermionlike properties—and, often, a Fermi surface with nonclassical exponents, and unusual exponents for correlation functions, but the correct “Luttinger” volume.

I will here restrict the term, for my purposes, to systems based on fermions—preferably ordinary electrons—and argue that the Luttinger liquid is a fixed point, or a manifold of fixed points, of the same renormalization group which, “usually,” leads to the Landau-Fermi liquid as a unique fixed point. (The interaction parameters of Landau-Fermi-liquid theory are well known² to be marginal operators around a single fixed point, the effectively free Fermi liquid.)

Some years before, Luther³ showed that the bosonization techniques used to solve these one-dimensional models are equally applicable to d -dimensional Fermi gases, and he claimed that they describe certain facts slightly more accurately than Fermi-liquid theory—the existence of $2k_F$ singularities in correlation functions, for instance, for the free-particle systems. But Luther did not consider the possibility that the interacting d -dimensional problem could lead to new physics.

The first new point I want to make is that two of the reasons usually given for the unique nature of one-dimensional Fermi systems are untenable. The first is that in 1D one has only forward scattering, or backward scattering where the momentum of one particle is maintained, if not its spin. This is indeed the correct reason for viability of the Bethe *Ansatz*. But after renormalization the Landau theory has only forward or exchange

scattering, and the renormalized particles indeed obey a Bethe *Ansatz* of the simplest form. This is the essence of Luther’s argument, that the excitations can be bosonized in each direction around the Fermi surface.

Second, it is argued that particles cannot be interchanged in 1D without encountering phase-changing interactions, and hence statistics are meaningless in 1D: but none of Haldane’s arguments seem to fail in the slightest if we introduce weak long-range hopping integrals in any of the examples, and such hopping integrals can allow a Berry process. No one argues, in fact, that real electrons living in 3D space in the presence of a chain of ions, which know perfectly well that they are fermions, will not obey the models and show the fractionization effects.

The unique effect in 1D is one which is also present in a class of higher- d models, specifically 2D repulsive Hubbard models, and in some strong-coupling higher- d cases. This is the presence of an *unrenormalizable Fermi-surface phase shift*. Such a phase shift signals that the addition of a particle changes the Hilbert space for the entire system of particles—it requires a net motion of field amplitude through the distant boundary of the system, or a net change of wavelengths. The effects of such phase shifts were explored thoroughly in connection with the “x-ray edge problem”⁴ and are summarized in the “infrared catastrophe” theorem:⁵

$$\langle VAC(V) | VAC(0) \rangle \propto \exp[-\frac{1}{2}(\delta/\pi)^2 \ln N], \quad (1)$$

where $|VAC(V)\rangle$ is the noninteracting Fermi sea in the presence of a potential V which causes a phase shift δ . The singularity is the result of the shifting of the entire spectrum of k values (in the presence of fixed boundary conditions) or of the displacement of wave-function nodes (for scattering boundary conditions), and is independent of the finite contribution which may ensue from local modifications of the wave functions.

In the conventional higher- d , free-electron-gas cases to which Landau-liquid theory applies, it is implicitly assumed—and indeed self-consistently so—that the phase shifts caused by adding or removing a single parti-

cle can be made to vanish in favor of a renormalization of all the quasiparticle mean-field energies. It is assumed that there is an effective mean-field energy whose eigenstates are the precise k states of the appropriate free-particle system.⁶ The formal result of this process is that the wave-function renormalization constant Z is finite: That is, the overlap integral

$$Z = \langle c_{k\sigma}^\dagger \Psi_G(N) | \Psi_{k\sigma}(N+1) \rangle > 0, \quad (2)$$

where Ψ_k is the exact wave function of the $(N+1)$ -particle state with one quasiparticle added, and in, particular,

$$\langle c_{k_F\sigma}^\dagger \Psi_G(N) | \Psi_0(N+1) \rangle > 0 \quad (3)$$

[where in a Fermi system, the $(N+1)$ -particle system necessarily has one particle added near the Fermi surface, and hence its ground state is quasidegenerate]. Equation (3) cannot be true if there is a phase shift due to the addition of $c_{k\sigma}^\dagger$.

In one dimension, for interacting particles, such a phase shift is unavoidable, since the effective range of interactions is necessarily (for real interactions) of the order of the wavelength ($\delta = k_F a$). Thus in all the realistic one-dimensional systems, $Z=0$, the Fermi-liquid fixed point is excluded, and the phase shifts due to interactions must be taken into account as relevant variables—in fact, in many cases renormalization invariants. $Z=0$ implies that the Fermi-sea excitations—which may still exist—do not carry charge (but may carry spin and be spinons). I will summarize Haldane's analysis of the spectrum of the 1D Hubbard model shortly.

In 2D, the scattering length for free particles and repulsive interactions diverges only as $1/k \ln k$ as $k \rightarrow 0$, and for higher dimensions it is $\sim 1/n \sim k_F^{-1/d}$; in both cases no serious problems need ensue for shorter wavelengths. But there is one type of problem where finite phase shifts are inevitable, namely, systems with a single-particle spectrum bounded above and below in energy. In this case the introduction of an extra particle may cause a bound state to split off from the top of the spectrum (an "antibound state").⁷ By Levinson's theorem,⁸ the presence of a bound state, either above or below the band, is signaled by a difference π in phase shift in the appropriate channel between top and bottom of the band. This corresponds to the fact that one state must be removed from the band to make up the bound state, and to Friedel's identity⁹

$$\Delta n(k) = \sum_l (2l+1) \delta_l(k) \quad (4)$$

for the change in number of states to be found below a wave vector k due to a phase shift $\delta(k)$. Continuity—or the fact that any bound state must be a superposition of all states in the band—tells us that some δ must remain finite at all energies in the band.

For any dimension, a repulsive interaction U sufficiently strong to split off an upper Hubbard band

adds one state to that band for each added electron; the "upper Hubbard band" can be thought of as equivalent to the manifold of antibound states and where it is present we must have $Z=0$ in the occupied lower Hubbard band, since the Hilbert space changes when we add a carrier. In the 2D Hubbard model (with one band, the generalized Hubbard models recently introduced are an irrelevancy) any repulsive potential whatever will split off bound states above the band, because of the well-known fact that in two dimensions all potentials bind. Thus, although for very low occupancies or very weak interactions the relevant singularities come in with small coefficients which are nonanalytic in interaction ($\sim e^{-1/u}$) or density ($e^{-n^2 \ln n}$), $Z=0$ in all cases. These terms will not be picked up in series expansions.

We can identify the relevant interactions by thinking of the upper Hubbard band as a kind of "ghost" condensate in a channel of $2k$ total momentum and zero total spin reflecting the fact that each particle of down spin prevents some state of the same momentum and up spin from being occupied, so that the "condensate" represents both states being occupied.

For each (conserved) total momentum $K = k + k'$, the final-state energy is a d -dimensional function of relative momentum Q which has some maximum value, above which the antibound state for momentum K appears for all U in two dimensions. Every scattering state in the K channel must be orthogonal to this state, which defines the eigenvalue of the S matrix which has finite phase shift. When we restrict ourselves to excitations near the Fermi surface by renormalizing away everything but a shell of states, there still must be a finite forward-scattering phase shift in the $K = 2k_F$ channel at each point in the Fermi surface. This finite phase shift means that up- and down-spin particles cannot occupy *exactly* the same k state. Thus, as in one dimension, one relevant interaction is forward scattering of up or down spins.

A second relevant interaction channel may be identified as the precisely backward scattering of up versus down spins, which comes from the $2k_F$ bound state of up-spin holes to down-spin electrons and vice versa; that is, the channel containing a $+k \uparrow$ electron and a $-k \downarrow$ hole. Viewed from the other hole-particle channel, this is a backward scattering.

It is worth discussing the resulting state in terms of a "renormalized Bethe *Ansatz*" picture. If we, following Benfatto and Gallivotti,² use a "poor man's renormalization-group" procedure to eliminate k states far from the Fermi surface, we will end up with a shell of low-energy excitations with momenta near the Fermi surface. Even if $Z=0$ and even in the presence of our new interactions, for the thin shell of states near k_F every real scattering is nondiffractive because of momentum conservation in that the two k -vectors never change: Charge is always scattered forward. When $Z=0$, however, the

original k states of the Fermi liquid are not adequate to contain all the particles, and the Bethe *Ansatz* wave function contains a continuous spectrum of k 's through the Fermi surface, exactly as in one dimension, where the large- U Hubbard model solution may be written

$$\sum_Q (-1)^Q \det \| e^{i k_r \cdot x_{Qj}} \| \times (\text{spin function}),$$

and the spectrum of k_r 's extends continuously to $|Q|$, $Q > k_F$. We presume that the same form is valid for renormalized particles in 2D, near the Fermi surface.

Under bozonization the backward-scattering interaction turns into a term proportional to $\nabla\theta_1\nabla\theta_1$ in the Hamiltonian for the phase-shift variables θ_σ , defined by $\nabla\theta_\sigma = 2\pi\rho_\sigma$. This term in the effective boson Hamiltonian must be transformed away by a Bogoliubov transformation. But as in one dimension, when transformed back into fermion variables the new dynamical variables, even though their equations of motion have linear dispersion relations, do not correspond to simple fermion or boson excitations, and have Green's functions with nonclassical exponents. They can be thought of as two spinless fermions (which is, after all, what we started with) two semions, or whatever; but all physical response functions correspond to fermion or boson combinations. Charge and spin separate, the low-energy spin excitations being like fermions at the original k_F , the charge excitations centering around the spanning vectors $2k_F$.

In a previous paper,¹⁰ we attempted to derive charge and spin separation by solving the double-occupancy problem with a slave-boson technique and a constraint; the basis of such a theory is undoubtedly correct but the mean-field treatment of the gauge variable, which results from the constraint, was not.

The actual correlation functions and Green's functions in the two-dimensional case have not yet been calculated: Fortunately, many experimental data can be calculated by using the photoemission data¹¹ to describe a semi-empirical fit, and by using the one-dimensional Hubbard model as an appropriate guide to understanding.¹² The actual calculation of physical properties will be described separately.

At present, all experimental observations seem compa-

tible with this point of view, and many puzzling ones receive almost unique explanations.

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⁶This is the essence of the procedure of A. A. Abrikosov, L. P. Gorkov, and I. Dzialoshinskii [*Methods of Quantum Field Theory in Statistical Mechanics* (Prentice-Hall, Englewood Cliffs, 1963), Sec. 20], which in the conventional case renormalizes the forward-scattering phase shift to $\delta \sim [\ln(\Delta\rho)]^{-1}$ by use of the Cooper phenomenon. This renormalization procedure cannot work if there are antibound states present, I presume, because the assumed "nonsingular" parts of the vertex are not harmless, but infinite.

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