"Confinement" in the One-Dimensional Hubbard Model: Irrelevance of Single-Particle Hopping

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We demonstrate, by direct use of the asymptotic Green's functions of Korepin and Ren, that the one-dimensional repulsive U Hubbard model has the property of "confinement," in that weak interchain coupling does not cause coherent particle motion in the transverse direction at absolute zero. Implications for real one-dimensional systems and for the two-dimensional Hubbard model are discussed.

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It is often assumed that an array of one-dimensional chains, weakly coupled by one-electron tunneling between chains, crosses over to two-dimensional behavior. We study this question for the repulsive Hubbard model and come to the conclusion that in this, and probably many other cases when the chain is not a Fermi liquid, the opposite is true: A finite interchain hopping is required. We call this behavior "confinement" because it has a close analogy to the confinement of quarks to the interior of the hadron. It is not quite equivalent to the usual Wilson definition of confinement.

The magnetic analogy of Heisenberg or Ising chains with weak interchain J has been of course well known to have the standard crossover behavior, in the Ising case since the time of Onsager. The interchain hopping case is suggested to be different by the existence of very large resistivity anisotropy in some materials, an observation which cannot be explained by anisotropic localization as it sometimes was in the past, since that is contrary to the theory of localization: An electron delocalized in one or two directions is simply delocalized.

The problem has not been very seriously attacked. A discussion by Wen [1] does not deal with the important issue of spin-charge separation, and one by Schulz [2] removes that separation by setting spin and charge velocities equal. Both Wen and Schulz also use a questionable criterion for relevance within the Fermi-liquid theory [3]. But actually, the main difficulty with these treatments is that the very concept of "relevance" may be itself irrelevant. At issue, as in the similar problem of localization, is coherence: the coherence or not of the tunneling process between the chains. In localization, there is no energy effect of the mobility edge, and conventional finite-temperature theory does not pick up the effect; here there are both energy and transport effects but the key is coherence.

Recent calculations [4–7] of the asymptotic one-particle Green's function at $T=0$ for the Hubbard model are sufficient to settle this question precisely. The interchain "hopping" is a simple static one-particle perturbation. The lowest-order response to it is given by a diagram involving creating a particle in one chain and a hole of equal momentum in a second, which do not interact except to recombine via the perturbation itself, so the response function is simply the product of the interacting electron and hole propagators, which to lowest order can be calculated exactly. We calculate the energy response but a simple identity would relate this to the conductivity.

It is instructive to do the noninteracting case first. The problem is not as simple as might appear at first. The relevant diagram (Fig. 1) leads to the response function

$$R = t_\perp^2 \sum_{k,\omega,\sigma} G_R^{1(e)}(k,\omega) G_R^{2(h)}(k,-\omega) ,$$

where 1 and 2 are separate Hubbard chains and we are calculating the response function to a perturbation connecting chains in an array of N chains i:

$$t_\perp \sum_i c_{k\sigma}^{\dagger(i)} c_{k\sigma}^{(i+1)} + \text{H.c.}$$

Note that R is also

$$2t_\perp^2 \int_{-\infty}^{\infty} dx \int_0^{\infty} dt\, e^{-\eta t} G_R^{(1)(e)}(x,t) G_R^{(2)(h)}(x,t) .$$

In general we should use the *retarded* Green's functions (designated by R) since we contemplate turning on the perturbation $t_\perp$ adiabatically at a rate $\sim\eta$ *after* any interactions are introduced on the separate chains. We are looking for an anomalous imaginary part to R representing real transitions, which signals a redistribution of electrons in k space.

The use of causal Green's functions will become the essential physical point when we consider the interacting chains, because we have to be very careful about the order of turning on the interactions U and $t_\perp$. We must realize that $U=0$ is a singular point at which the nature of the spectrum changes qualitatively, so that we cannot expect that turning on $t_\perp$ and then U will have the same result as the opposite order. Even though some results may be obtained with renormalization methods from per-

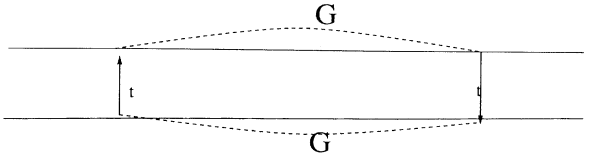

FIG. 1. Lowest-order diagram for interchain tunneling.

turbation theory in U for the original problem with $t_\perp = 0$ we should be reasonably sure that confusing the order by using time-ordered Green's functions and not retarded ones will be incorrect. If we first go to finite, large U, where the spectrum is qualitatively different from near-zero U—having spin-charge separation, in particular —and then turn on $t_\perp$ and/or T as small perturbations, we find quite different results from those given by the standard temperature Green's functions.

Figure 2 illustrates the problem. On the vertical axis we have the perturbation $t_\perp$ (actually the same diagram holds true for a number of types of T-invariant perturbations). On the horizontal axis is U. We intend to show that a line A separates the region where $t_\perp$ is irrelevant from that where it causes finite tunneling or other effects. Clearly, to reach region B below line A, we must *first* turn on U and then $t_\perp$; if we go in the opposite order, which is implied by conventional procedures, we shall end up in region C, and will miss the effect. Thus it is essential to maintain the time ordering of events. Clearly $t_\perp = 0$, $U = 0$ must be a singular point at which Fermi-liquid theory starts to fail.

If we first turn on $t_\perp$ we know easily what will happen physically. $t_\perp$ will split the unperturbed energy levels ϵ_k into a two-dimensional manifold; for a simple pair of chains 1 and 2 we will get $\epsilon_k \rightarrow \epsilon_k \pm t_\perp$, the two energies belonging to symmetric and antisymmetric linear combinations. Thus the Fermi surface will shift to $k_F \rightarrow k_F \pm t_\perp/\hbar v_F$ and, to lowest order in U, we will have no singular scatterings from $k_F + t_\perp$ to $k_F - t_\perp$ and the system will be effectively two roughly independent different Hubbard-like models with smaller effective U. If we introduce many chains there will be a two-dimensional Fermi surface and a whole new two-dimensional problem to solve. The energy response is of order $t_\perp^2$ because $\sim t_\perp$ levels have been shifted by $\sim -t_\perp$ by reoccupation; without a shift of Fermi surface there would be no response.

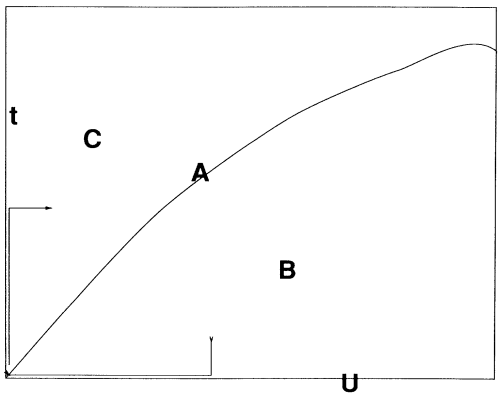

FIG. 2. Proposed $t_\perp$-U phase diagram. A represents a boundary between one and two-dimensional behavior. One cannot reach the "confined" regime B perturbatively by the path of turning on $t_\perp$ and then U.

The most straightforward way of approaching this problem seems to lead to nonsense: no response. (The argument is foreshadowed by Kohn and Luttinger [8].) We have

$$R = t_\perp^2 \sum_k \int_0^\infty d\omega\, G_e(k,\omega) G_h(k,-\omega)\,,$$

$$G_e(k,t) = \langle 0 | c_k(t) c_k^\dagger(0) | 0 \rangle = e^{i\epsilon_k t - \eta t}(1-n_k)\,,$$

$$G_h(k,t) = e^{-i\epsilon_k t - \eta t}(n_k)\,,$$

$$G_e(k,\omega) = \frac{1-n_k}{\omega - \epsilon_k - i\eta}\,, \quad G_h = \frac{n_k}{\omega + \epsilon_k + i\eta}\,,$$

where $\epsilon_k = \hbar v_F(k - k_F)$ and η defines outgoing boundary conditions for the causal Green's function. Clearly, at $T = 0$, $n_k(1-n_k) \equiv 0$ and there is zero response. This reflects correctly the fact that without readjustment of populations, there is in fact no net energy shift.

This anomaly is traditionally converged by introducing finite temperature. If

$$n_k = f(\beta\epsilon_k)\,,$$

we get, from either the frequency or the time representation,

$$R = t_\perp^2 \sum_k n_k(1-n_k)\frac{1}{2\eta} \sim \frac{t_\perp^2 N(0) T}{\eta}\,.$$

The response diverges with $1/\eta$, reflecting the coincidence of two singularities "pinching" from opposite sides of the real axis. In the time domain, this η singularity is obvious:

$$R = t_\perp^2 \sum_k \int_0^\infty dt\,(n_k)(1-n_k) e^{-2\eta t} = t_\perp^2 \sum_k n_k \frac{1-n_k}{2\eta}\,.$$

The perturbation *for each* k acts for an infinite time and is converged only by the artificial factor η. The Matsubara perturbation technique allows us to "fuzz out" the energies ϵ_k by moving the poles off the real axis by an amount T, and one gets the right answers, at least for $t \ll T$, for a devious reason which was explored within Fermi-liquid theory by Kohn and Luttinger and by Bloch and deDominicis. But as they show, such singularities proportional to $1/\eta$ are the signal for Fermi surface shifts, for rather obvious reasons as pointed out above.

Now we are ready to approach the interacting problem correctly. After we turn on U, the space-time Green's function becomes, asymptotically,

$$G_e \sim e^{ik_F x} \frac{1}{[(x - v_s t)(x - v_c t)]^{1/2}} \frac{1}{(x^2 - v_c^2 t^2)^\alpha} + e^{-ik_F x}(x \rightarrow -x), \quad 0 < \alpha < \tfrac{1}{16}\,;$$

for G_h, $t \rightarrow -t$. There is a multiplicative factor involving an energy cutoff $\sim \Lambda \sim \hbar v_F/a$, of order $2\alpha\Lambda^{2\alpha}$.

Fourier transforming this structure is difficult [9]. An approximation which loses none of the essential physics is to take advantage of small α and large U (for which $v_c/v_s \gg 1$) to treat the terms $(x^2 - v_c^2 t^2)^{-\alpha}$ as a slowly varying, logarithmlike term which simply multiplies by convergence factors $(iv_c t)^{-2\alpha}$ or $x^{-2\alpha} \sim (k - k_F)^{2\alpha}$, whichever is smaller.

Then we can get an adequate approximation to $G(k,t)$. Define $\Delta k = k - k_F$, $\bar{v} = \frac{1}{2}(v_c + v_s)$, and $\Delta v = v_c - v_s$; then

$$G_e(k,t) = \int dx\, e^{-ikx} G_e(x,t)$$
$$\propto e^{-\eta t} n_k e^{i\bar{v}\Delta k t} J_0(\Delta v\, \Delta k\, t)(iv_c t)^{-2\alpha}.$$

It is clear that now the convergence factor η is essentially irrelevant; even at k_F, $t^{-2\alpha}$ or $\Delta k^{+2\alpha}$ provides a convergence factor, and everywhere else J_0 falls off as $t^{-1/2}$. The reason is the conversion of the Fermi-liquid pole into a cut along the real axis, or physically the fact that charge and spin do not propagate with the same velocity; hence the singular perturbation has no chance to act. This is why the result is qualitatively different for the system with spin. The response to our perturbation then works out roughly as

$$R \propto t^2 \sum_k n_k(1 - n_k) \int \frac{dt\,(\Delta k)^{2\alpha}}{t^{2\alpha} \Delta v\, \Delta k\, t} e^{-2\eta t}.$$

It looks as though our convergence factor is being used twice but we believe this expression gives the right convergent behavior. There is indeed an energy response, but it is small and entirely due to virtual hopping, not real transitions, as we see by the fact that the convergence factor η does not enter the answer.

Formal theory at finite temperature seems to be difficult; the crude holon-spinon ideas we have suggested in the past may be the best way to show that at finite T or frequency there is a T-linear conductivity between chains; this could also be done by gauge methods.

This answer should not be at all unexpected. As we have repeatedly emphasized, the Luttinger liquid of the Hubbard model is an incompressible spinon liquid, if we think of spinons as the limiting case as $Z \to 0$ of electron quasiparticles (the so-called marginal Fermi-liquid concept, proposed in [10]), and we recognize that if in the Luttinger liquid, as shown by the exact Lieb-Wu solution, the spinon Fermi velocity is finite, this must mean that the self-energy as we approach this limit obeys

$$v_s = \frac{\partial \Sigma / \partial k}{\partial \Sigma / \partial \omega} = \text{finite}.$$

But if $\partial\Sigma/\partial\omega \to \infty$, this means $\partial\Sigma/\partial k \to \infty$, which implies that the spinon liquid is incompressible:

$$K = \frac{K_0}{1 + \partial\Sigma/\partial k} \to 0.$$

The spinon gas cannot change density without exciting a second type of excitation, the holon, which plays the role of a density of sites which the spins may occupy. Again, spin is vital, as is the existence of two different velocities. This means that one-particle perturbations cannot shift the Fermi level in momentum space, which prevents electrons tunneling into and out of the liquid. We hope to show in a later work that the same is true of impurity potentials: The liquid is immune to spin-independent potentials, and hence has infinite conductivity (and does not localize) even in the presence of impurities. And, of course, since we have shown that $Z \to 0$ in the 2D Hubbard model, all these properties hold in that case as well. (Confinement is also expected to hold for 2D quantum Hall systems—see the results of Boebinger [11].)

It is often argued that renormalized perturbation theory (so-called "g-ology") is an adequate method to obtain properties of one-dimensional models, in particular, the Hubbard model. Although some details differ from the more complete bosonization [6] or "Luttinger-liquid" method [12] these seemed irrelevant to many. After 20 years of g-ology, however, we now see that these responses are different from the conventional assumptions based on perturbation theory.

The immediate result is relevant for a number of "1D" systems. It seems likely that the extension to negative U, and certainly to the t-J model, is straightforward, and that if such systems take on a 1D correlated liquid state they may confine in the other two directions. The "organic superconductors," however, are in general 2D systems and we expect 2D confinement to occur in some of these, if not all. We suspect that data on transport in these systems will reward reexamination from a fresh point of view.

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