Localization of a defect in a 1D electron gas

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(Submitted 20 February 1995)
Pis'ma Zh. Éksp. Teor. Fiz. **61**, No. 8, 636–642 (25 April 1995)

The localization of an impurity due to backscattering by the impurity potential of a 1D interacting electron gas is analyzed. The argument of the exponential function is calculated for the orthogonality integral corresponding to a displacement of the scattering potential by an arbitrary distance. It is shown that the "orthogonality catastrophe" due to backscattering can be arbitrarily large. The results derived here depend strongly on the interaction in the system. They are fundamentally different from those in the case of noninteracting electrons and also from the existing results for 2D and 3D systems. © *1995 American Institute of Physics.*

1. One-dimensional (1D) systems have attracted interest because of the real technological possibility of creating such systems in semiconductor nanostructures, because of research on the properties of organic conductors, and also because of direct applications in describing the low-temperature dynamics of systems under conditions of the quantum Hall effect. A system of interacting electrons in 1D has several properties which have no analogs in spaces of higher dimensionality. In particular, as was shown in Refs. 1, any impurity potential, no matter how weak, in a system of electrons with repulsion asymptotically leads to total reflection from the potential, because of an intensification of backscattering. From the conductivity standpoint, the system thus becomes an insulator at $T=0$. The backscattering of an electron (with a momentum change of $2k_F$) also alters the power-law singularity in the intensity of the emission/absorption of a photon near the threshold. In the 2D and 3D cases, the photoabsorption intensity has a behavior $I(\omega) \propto \omega^{\alpha}$, with an exponent α which depends explicitly on the properties of the scattering potential of a hole which arises in an inner atomic shell as the result of a transition of an electron into the conduction band.[2] In a 1D system, backscattering leads to a universal value of the exponent α. This value remains finite even if the scattering potential and electron correlations tend toward zero.[3]

The results found previously were derived under the assumption that the scattering potential remains a *static* potential. Since the response is singular after a long time, the validity of this assumption requires that the scattering center be localized in its ground state. As we show below, this condition is met only under certain other conditions. In general, we are dealing with the mobility of a defect of an arbitrary nature in the 1D case and a calculation of the response of the system to a dynamic potential if the defect becomes delocalized.

We assume that the scattering particle, in addition to interacting with conducting

electrons, is in a periodic potential of a lattice and that its kinetic energy is described by the tight-binding model:

$$H_h=\Delta\sum_n d_{n+1}^{\dagger}d_n+\text{h.c.}, \tag{1}$$

where the operator $d_n^{\dagger}$ creates a particle at site n, and the hopping matrix element Δ is assumed to be small in comparison with the Fermi energy E_F (the Fermi energy also plays the role of a characteristic high-frequency cutoff in the problem).

The system of electrons is described in terms of a Luttinger liquid.[4] In second quantization, the Hamiltonian of a spin-zero Luttinger liquid is[4]

$$H_0=\sum_q \omega_q b_q^{\dagger}b_q+\frac{\pi}{2L}(v_N N^2+v_J J^2), \tag{2}$$

where $\omega_q\approx c|q|$ at small values of the wave vector $q=2\pi k/L$ (k is an integer), $L\to\infty$ is the length of a chain, and N and J are integers, equal to respectively the total number of particles (counted from the ground state) and the difference between the numbers of electrons moving to the right and to left. The velocities associated with the charge excitations, $Q=eN$, and the current excitations, $j=ev_J/L$, depend on the sound velocity c and the electron–electron coupling constant g. We therefore have $v_N=c/g$ and $v_J=cg$. The value $g=1$ corresponds to a free gas, while values $g<1$ correspond to a repulsion between particles.

Corresponding to forward scattering is a local interaction with fluctuations in the electron density, $H_F=V_F\Psi^{\dagger}(x)\Psi(x)$, or

$$H_F=\sqrt{g}V_F\sum_q \sqrt{\frac{|q|}{2\pi L}}(b_q+b_{-q}^{\dagger})e^{-iqx}. \tag{3}$$

The backscattering of an electron, $H_B=V_B\Psi_l^{\dagger}(x)\Psi_r(x)+\text{h.c.}$ changes the number J by 2 and simultaneously leads to the excitation of density fluctuations. In the boson representation, the Hamiltonian H_B can be rewritten as[5]

$$H_B=\sum_{J=-\infty}^{+\infty}(V_B e^{2ik_F x}a_{J+2}^{\dagger}a_J e^{\sqrt{g}S}+\text{h.c}), \tag{4}$$

$$S=i\sum_{q\neq 0}\text{sgn}(q)\sqrt{\frac{2\pi}{|q|L}}(b_q+b_{-q}^{\dagger})e^{-iqx}. \tag{5}$$

Here S is the standard shift operator for normal oscillators. This Hamiltonian is identical to the Hamiltonian of a particle on a lattice which is interacting with an ohmic boson heat reservoir[6]—a problem which has been examined quite closely over the past few decades (Ref. 7, for example).

To resolve the question of a localization of a scattering particle in the ground state we need to find the argument of the exponential function for the orthogonality integral between states of the system which correspond to scattering by the potential at the points $x=0$ and $x=a$, respectively:

$$\langle V(x=0)|V(x=a)\rangle \equiv e^{-\phi} \sim \exp\{-K\ln(E_F/E_{\min})\}. \tag{6}$$

When K is above a critical value $K_c=1$, the particle becomes localized in the lattice at $T=0$, despite the translational symmetry of the problem[8,7] (at least in the approximation quadratic in Δ; see also the discussion below). The localization question can be discussed quite easily by taking the following simple approach. The interaction of a particle with the reservoir leads to a polaron contraction of the effective hopping amplitude in accordance with

$$\bar{\Delta}=\Delta e^{-\phi}=\Delta[\bar{\Delta}/E_F]^K. \tag{7}$$

We have introduced a self-consistent cutoff at low energies, since over times $t\bar{\Delta}>1$ we can no longer treat the scattering by the potential as static. At $K<1$ the solution of the self-consistent equation

$$\bar{\Delta}=\Delta[\Delta/E_F]^{K/(1-K)} \tag{8}$$

determines an energy scale below which a particle becomes delocalized. At $K\geqslant 1$, the unique solution of Eq. (8) is $\bar{\Delta}=0$.

2. We first consider forward scattering. In this case the potential at the point $x=a$ contains an additional phase factor $\exp\{-iqa\}$, not present in the case $x=0$. Using the standard transformation which diagonalizes H_0+H_F, we find

$$e^{-\phi_F}=\exp\left\{-\frac{g\delta_F^2}{2\pi^2}\int_0^{q_{\max}}\frac{dq}{q}(1-\cos qa)\right. . \tag{9}$$

The integral over dq is well defined in the limit $q\to 0$, and the infrared singularity is cut off at $q\sim 1/a$ (here $\delta_F=\pi V_F/c$). Consequently, forward scattering leads to only a finite renormalization of the hopping amplitude, because of processes at high energies, to a certain value $\bar{\Delta}=\Delta e^{-\phi_F}$. At low temperatures the particle thus becomes delocalized. It would seem that this delocalization would lead to a spreading of the singularity in the photoabsorption spectrum. However, in the 1D case, long-wave fluctuations of the density are scattered forward by a moving particle, as at a fixed center. The dynamics of a particle can be ignored if the size of the delocalization region is much smaller than the reciprocal of the momentum transfer in a typical scattering event. By the time t, the length scale of the delocalization of the particle is at best no greater than $l<v_g t$, where v_g is the maximum group velocity [for a quadratic dispersion relation, $\epsilon(p)=p^2/2M_*$, coherent delocalization of a wave packet does indeed occur by the vastly slower law $l^2\sim t/M_*$]. The singularity in $I(t)$ is due primarily to wave vectors $cqt\sim 1$. As a result, the necessary condition $ql\ll 1$ holds at all times, and the power-law singularity due to forward scattering does not depend on the motion of the particle.[9]

This result is sharply at odds with the conclusion which follows from the delocalization of a center in the 2D or 3D case or when backscattering is taken into account in 1D. In all these cases the infrared singularity is associated with *large* values of the momentum transfer at *low* energies. For a short-range potential, the infrared singularity is determined by integrals of the type $\int_{FS}d\mathbf{q}\int dE/E$. If we assume a coherent delocalization of the particle after a long time, then we are left with only the contribution of small

values of the momentum transfer at $t\to\infty$: $|q|^2\sim M_*/t$. The resultant contribution of these small values to the orthogonality integral falls off with increasing t in accordance with

$$K\sim\begin{cases}1/T_0t, & \text{3D},\\ 1/\sqrt{T_0t}, & \text{2D},\\ 0, & \text{1D (backscattering)},\end{cases} \tag{10}$$

where $T_0=M_*k_F^2$, and Eq. (10) is valid under the condition $T_0t\gg 1$. This conclusion agrees completely with the arguments of Nozieres.[10]

There is also a purely kinematic factor which forbids scattering through a large angle at low energies. We note that T_0 agrees with the typical recoil energy in quasielastic scattering of an electron. Let us assume that the energy of the particle is much smaller than T_0 and that the incident electron has an energy $\epsilon-\epsilon_F\ll T_0$. Under these conditions, scattering with a transfer $q\sim k_F$ is forbidden by the Pauli principle, since the maximum possible energy transfer is much smaller than T_0. We are left with only small-angle scattering of electrons near the Fermi surface. A simple estimate shows that the area of the Fermi surface which is covered by the allowed final states of the electron falls off in proportion to the square of the momentum of the particle: $K\sim p^2/k_F^2$. We thus go back to Eq. (10). In the 2D, 3D, and 1D cases the infrared divergence is thus smeared for the case of backscattering if the scattering center is delocalized over a length scale $l>1/k_F$.

3. We now consider conditions under which the argument K in (6) is greater than the critical value of one. In 2D and 3D, this condition can be satisfied only for a sufficiently long-range potential, which has several orbital scattering channels which contribute to the orthogonality integral. The exact expression for K is[11]

$$K=\frac{1}{8\pi^2}\mathrm{Tr}\{\ln^2[S^{-1}(a)S(0)]\}=\frac{1}{2\pi^2}\sum_j(\delta_j^{\mathrm{eff}})^2, \tag{11}$$

where $S(a)$ is the S-matrix for scattering by the potential $V(a)$, and the effective scattering phase shifts determine the eigenvalues of the matrix, $[S^{-1}(a)S(0)]_{jj}=e^{-2i\delta_j^{\mathrm{eff}}}$. In general, $S(a)$ and $S(0)$ do not commute. For an arbitrary potential there is a theorem[12] which restricts the phase shifts to certain values: $|\delta_j^{\mathrm{eff}}|\leq\pi/2$. This restriction means that we need more than eight nonzero eigenvalues $\{\delta_j^{\mathrm{eff}}\}$ (more than four when spin degeneracy is taken into account) in order to reach the critical value $K_c=1$. At first glance, the localization of a particle due to backscattering would seem impossible in principle in 1D, since the only scattering mechanism in the original potential leads to at best two nonzero effective scattering phase shifts, so their resultant contribution would not exceed 1/4. This assertion is indeed correct for a free electron gas, but the behavior of an interacting system completely contradicts the intuition developed at a higher dimensionality. Under the condition $g<1$, the contribution of fluctuations of the spin and charge densities to the orthogonality integral is *zero*! (In 2D and 3D, the orthogonality integral is determined exclusively by density fluctuations.) For a short-range and otherwise arbitrary potential, regardless of the position of the scattering center, we have the

same state of the electron subsystem, corresponding to complete reflection from the potential (the electron phase shift in the even and odd channels are respectively $\pi/4$ and $-\pi/4$; Ref. 3).

A nonzero contribution to (6) arises not from a continuum of excitations of electron–hole pairs but from a single degree of freedom, associated with the quantum number J. The orthogonality catastrophe is stronger than that for a free gas. In representation (4), a displacement of the scattering potential to a neighboring position $x=a$ changes the phase of the backscattering amplitude: $V_B \rightarrow V_B e^{2ik_F a}$. From the standpoint of the variable J, the additional phase shift in the hopping amplitude $J \rightarrow J+2$ is equivalent to a shift of the center of the Brillouin zone in the momentum representation to the point $P_J = k_F a$. The obvious unitary transformation

$$\tilde{H} = e^{ik_F aJ} H e^{-ik_F aJ} \tag{12}$$

links the states of the system before and after the shift of the potential. The orthogonality integral can now be described by the expression

$$e^{-\phi_B(t)} = \langle e^{ik_F aJ(0)} e^{-ik_F aJ(t)} \rangle = \exp\left(-\frac{(k_F a)^2}{2} \langle J(0)J(t) \rangle \right). \tag{13}$$

We now make use of some existing results for the dynamics of a particle which is interacting with an ohmic reservoir. Under the condition $g<1$, the ground state of the variable J is delocalized with $\langle J^2 \rangle \gg 1$. Actually, the pronounced uncertainty in the current state of a 1D system (the current operator is $v_J J/L$; Ref. 4) is identical to the assertion that there is a complete reflection of excitations from the potential.[5] In the continuum limit of large J, the correlation function in Eq. (13) can be expressed in terms of the mobility in accordance with[8] $\langle J(0)J(t) \rangle \sim 2/(\pi^2 g) \ln t$. As a result, we find

$$K = \frac{1}{g} \left(\frac{k_F a}{\pi} \right)^2 \quad (|k_F a| \leq \pi/2). \tag{14}$$

This result was derived in Ref. 13 for the case $2k_F a = \pi$ (a change in the sign of the potential). Since J is discrete, expression (14) should be continued periodically for $|k_F a| > \pi/2$. Unexpectedly, the orthogonality of the states of the system under a shift of the potential is determined by a restructuring of a single mode of the medium. In the case $g \rightarrow 0$, the argument of the exponential function can be arbitrarily large.

Under the condition $g < (k_F a/\pi)^2$, the dynamics of the scattering center is thus frozen at $T=0$, and the infrared singularity is retained in the backscattering (in particular, the chain becomes an insulator at $T=0$). We should point out here that the arguments above were based on an analysis of the effective amplitude for a hop between nearest positions, $n \rightarrow n+1$. If the corresponding argument $K_{n,n+1} \equiv K_1$ is greater than one, the amplitude for a hop to a neighboring site can be ignored in the low-temperature limit. This assertion does not, however, mean that we can also ignore transitions to the next-nearest site (or, in general, transitions over several sites): $n \rightarrow n+m$ with $m \geq 2$. Such transitions were originally negligible: $\Delta_m \sim \Delta^m / W^{m-1} \ll \Delta$. The corresponding argument in the scaling, $K_m = 1/g(k_F ma/\pi)^2$ ($|k_F ma| \leq \pi/2$), can be less than one at a certain value of m, since we are dealing with a periodic function of m, and k_F is generally not commensurate with $1/a$. This statement means that in the limit $L \rightarrow \infty$ a particle will

unavoidably become delocalized at an energy scale determined by the largest of the self-consistent solutions $\overline{\Delta_m}$ (which probably corresponds to the smallest value of m for which the condition $K_m < 1$ holds). In real systems, this energy scale is probably of purely academic interest for $m \geqslant 2$. By way of comparison we note that in the standard dissipative model (as is the case for the variable J) (Refs. 6–8) the dependence $K_m \propto (ma)^2$ is assumed to be valid for all values of ma, so the localization condition $K_1 \geqslant 1$ automatically means that *all* the hopping amplitudes are zero in the ground state.

4. We now consider the completely different case in which the infrared divergence persists in the backscattering processes to extremely low energies for a *mobile* center. We assume that the constant for the interaction between electrons satisfies the condition $1/4g \gg 1$ at a small value of the Fermi momentum, $k_F a \ll 1$, so the argument of the exponential function in the orthogonality integral between nearest neighbors, (13), is smaller than the critical value (or even the condition $K_1 \ll 1$ holds). At a temperature $T < \bar{\Delta}$, determined by Eq. (8), the particle becomes delocalized and acquires an effective mass on the order of $1/\bar{\Delta}a^2$. Assuming a coherent delocalization at lower temperatures, and applying the same arguments regarding the scattering of electrons through a large angle as in the derivation of (10), we would find a smearing of the infrared divergence at energies below $T_0 \sim \bar{\Delta}(k_F a)^2$. However, a coherent delocalization at the scale T_0 is not possible if the parameter g is small. At temperatures above T_0 (at which the momentum of the particle is much greater than k_F), a calculation of the scattering probability Γ in the standard ohmic model, which corresponds in our case to quasielastic scattering of electrons by a particle, yields[14]

$$\Gamma = T_0 \frac{2}{\pi g}. \tag{15}$$

We see that we have $T_0 \ll \Gamma < \bar{\Delta}$ for small values of g, while at temperatures $T < \Gamma$ a coherent dynamics of the particle is impossible in principle. Under these conditions a wave packet spreads out logarithmically:

$$k_F^2 \langle (R(0) - R(t))^2 \rangle \sim \frac{g}{2} \ln \Gamma t. \tag{16}$$

In contrast with the corresponding result for the variable J, which was valid at all T, expression (16) is good only as long as its right side is less than one. Nevertheless, up to exponentially long times $t_o \sim \Gamma^{-1} e^{2/g}$, the scattering of electrons by the particle does not differ from scattering by a static center. Only at times $t > t_o$ does the length scale of the delocalization of the particle begin to exceed $1/k_F$, and only at such times are the infrared divergences smoothed over.

In summary, at values $g \ll 1$ the singular properties of the backscattering process are seen in their full glory in the spectrum of the photoabsorption/emission and in the conductivity, regardless of whether the argument of the exponential function in the orthogonality integral between nearest sites has the critical value of one.

This study was supported by the Russian Fund for Fundamental Research (95-02-06191a) and, partially, by the Canadian Research Foundation NSERC and the Laue–Langevin Institute.

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Translated by D. Parsons