RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 49, NUMBER 3 15 JANUARY 1994-I

Fermi-edge singularities and backscattering in a weakly interacting one-dimensional electron gas

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(Received 24 August 1993)

The photon-absorption edge in a weakly interacting one-dimensional electron gas is studied, treating backscattering of conduction electrons from the core hole exactly. Close to threshold, there is a power-law singularity in the absorption, $I(\epsilon) \propto \epsilon^{-\alpha}$, with $\alpha = \frac{3}{8} + \delta_+/\pi - \delta_+^2/2\pi^2$, where δ_+ is the forward-scattering phase shift of the core hole. In contrast to previous theories, α is finite (and universal) in the limit of weak core-hole potential. In the case of weak backscattering $U(2k_F)$, the exponent in the power-law dependence of absorption on energy crosses over to a value $\alpha = \delta_+/\pi - \delta_+^2/2\pi^2$ above an energy scale $\epsilon^* \sim [U(2k_F)]^{1/\gamma}$, where γ is a dimensionless measure of the electron-electron interactions.

The understanding of the nature of the singularities in the x-ray-absorption edge in metals has played an important role in modern condensed matter physics.[1,2] With the advent of new microelectronics technology it has become possible to study the related Fermi-edge singularities in one-dimensional (1D) quantum wires.[3] Since in one dimension electron-electron interactions destroy the Fermi surface, it is an important problem to understand how the combined effects of reduced dimensionality and interactions affect the qualitative nature of the edge singularities.

In 3D metals, the power-law singularity in the absorption edge is determined by the famous relation

$$I(\epsilon) \propto \left(\frac{D_0}{\epsilon}\right)^{\alpha} \theta(\epsilon), \tag{1}$$

with the exponent α given by

$$\alpha = 2\delta_0/\pi - \sum_l (\delta_l/\pi)^2. \tag{2}$$

Here $\epsilon = \hbar(\omega - \omega_{\rm th})$ is the energy of a photoelectron counted from the Fermi level, $\omega_{\rm th}$ is the absorption threshold frequency, D_0 is the conduction electron bandwidth, and δ_l are the scattering phase shifts associated with the core hole seen by electrons at the Fermi energy. It is assumed that $l = 0$ is the dominant channel. In a noninteracting 1D electron gas, there are two phase shifts, δ_e and δ_o, corresponding to wave functions which are even and odd about the origin. It is more convenient to introduce linear combinations of these phase shifts, $\delta_\pm = \delta_e \pm \delta_o$. In this representation, the result (2) has the form

$$\alpha = \frac{\delta_+ + \delta_-}{\pi} - \frac{\delta_+^2 + \delta_-^2}{2\pi^2}. \tag{3}$$

In the Born approximation, the new phase shifts are related to two different Fourier components of the core-hole potential $U(q)$,

$$\delta_+ = \frac{U(0)}{\hbar v_F}, \quad \delta_- = \frac{U(2k_F)}{\hbar v_F}, \tag{4}$$

where v_F and k_F are the Fermi velocity and the wave vector.

Recently, a number of authors[4,5] have addressed the effect of electron-electron interactions in 1D metal in a simplified model with $U(2k_F) = \delta_- = 0$. They concluded that the power-law structure survives with an exponent modified by the interactions. However, α remains small if the scattering potential $U(0)$ is weak.

In this paper we show that even a small $2k_F$ scattering changes this result *qualitatively.* In particular, the exponent in Eq. (1) always becomes of order of 1 in the immediate vicinity of the threshold energy. The growth of α at low energies is caused by the interaction-induced renormalizations[6,7] of $2k_F$ scattering that increase the effective value of $U(2k_F)$ and, correspondingly, of δ_-. The quantitative behavior of $\delta_-(\epsilon)$ can be found in the case of weakly interacting electrons, when it is possible to define the transmission amplitude t and to relate it to the phase shifts by a standard scattering theory formula,

$$t = e^{i\delta_+} \cos\delta_-. \tag{5}$$

In the limit of weak interaction, the renormalized transmission amplitude can be found[8] at any energy,

$$t(\epsilon) = \frac{t_0(\epsilon/D_0)^\gamma}{\sqrt{|r_0|^2 + |t_0|^2(\epsilon/D_0)^{2\gamma}}}, \tag{6}$$

where $|r_0|^2 = 1 - |t_0|^2$ is the bare reflection coefficient, and $\gamma \equiv [V(0) - V(2k_F)]/2\pi\hbar v_F$ is determined by the Fourier components $V(q)$ of the electron-electron interaction potential. Comparing (5) with (6) we conclude that δ_+ does not depend on energy and corresponds to the unrenormalized value of the transmission amplitude t_0. In agreement with Ref. 7, transmission amplitude vanishes at low energies which implies saturation of the other phase shift at $\delta_- = \pi/2$. Consequently, according to Eq. (3), very close to the threshold the exponent α is given by

$$\alpha = \frac{3}{8} + \frac{\delta_+}{\pi} - \frac{\delta_+^2}{2\pi^2}. \quad (7)$$

Thus, α near the threshold differs from the results of works[4,5] by 3/8. The region of energies where Eq. (7) is valid depends on $U(2k_F)$. For a weak backscattering, there is a clear crossover between the values given by (7) and the results of Refs. 4 and 5, as shown in Fig. 1. This crossover occurs at the energy scale ϵ^* where the phase δ_- becomes of the order of 1. Using Eqs. (5) and (6), we find

$$\epsilon^* \sim D_0 \left|\frac{r_0}{t_0}\right|^{1/\gamma} \sim D_0 \left|\frac{U(2k_F)}{\hbar v_F}\right|^{1/\gamma}. \quad (8)$$

The simple picture presented above has two drawbacks. It uses Eqs. (1) and (5) that are valid, strictly speaking, for noninteracting electrons only. Besides, Eq. (2) assumes energy-independent phase shifts.

In order to establish the above results, it is necessary to develop an approach that treats both the renormalizations of δ_- and the absorption intensity $I(\epsilon)$ in a unified manner. For noninteracting electrons, a number of techniques have been used to this end. Nozieres and de Dominicis[2] summed the perturbation series in the strength of the potential. Ohtaka and Tanabe used a technique based on Slater determinants.[9] Schotte and Schotte employed a bosonization technique.[10] The latter approach is the most natural to generalize when including electron-electron interactions.

Bosonization has proved a very useful technique for studying the interacting 1D electron gas, or Luttinger liquid.[11] The advantage of bosonization is that in the absence of backscattering, the low energy behavior is determined by a free field theory, which describes the collective density fluctuations, and exact results for the behavior of correlation functions may be simply obtained. Unfortunately, backscattering of electrons will introduce a nonlinear term into the theory which cannot be treated exactly. Schotte and Schotte employed a different bosonization scheme, however, which allowed them to treat exactly the scattering of 3D noninteracting electrons on a core hole.[10] They applied the bosonization technique to each angular momentum channel independently. We use a similar approach for our 1D problem that allows us to treat the backscattering potential exactly.

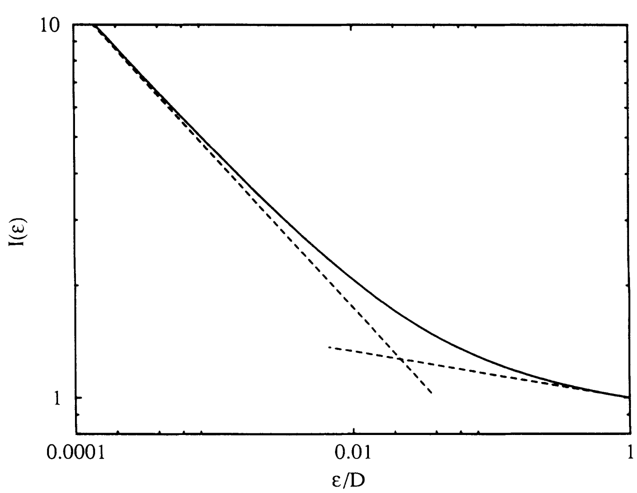

FIG. 1. A log-log plot showing the crossover in the x-ray response obtained by numerically integrating Eq. (21). We have set $\gamma = 0.6$, which is the correct order of magnitude for a GaAs quantum wire. The core-hole potential is characterized by $\delta_+ = 0.1$ and $\delta_-(0) = 0.1$. The dashed lines indicate the asymptotic power laws for $\epsilon \ll \epsilon^*$ and $\epsilon \gg \epsilon^*$, with $\epsilon^*/D \approx 0.02$.

Here we briefly outline this nonstandard bosonization transformation. For $k > 0$, instead of usual left (L) and right (R) movers described by wave functions $e^{\pm ikx}$ we introduce even (e) and odd (o) channels corresponding to $\cos kx$ and $\sin kx$, respectively. The electron annihilation operators corresponding to these states are then related by $\psi_{L,R}(k) = [\psi_e(k) \pm i\psi_o(k)]/\sqrt{2}$. We then define bosonic fields $\phi_{e,o}(\tilde{x})$ such that

$$\tilde{\nabla}\phi_{e,o}(\tilde{x}) = \sum_{k,q} e^{iq\tilde{x}} \psi_{e,o}^\dagger(k+q)\psi_{e,o}(k). \quad (9)$$

(Note that the coordinate $\tilde{x}$ should not be confused with the physical coordinate x, since the transformation to even and odd wave functions mixes x and $-x$.) We may then, as usual, express the electron creation operator as

$$\psi_{e,o}(k) = \frac{1}{\sqrt{2\pi\eta}} \int_{-\infty}^{\infty} d\tilde{x} e^{-ik\tilde{x}} \exp[i\phi_{e,o}(\tilde{x})], \quad (10)$$

where $\eta \approx \hbar v_F/D_0$ is the short distance cutoff. When expressed in terms of these variables, the Hamiltonian for noninteracting electrons, including backscattering, is quadratic in $\phi_{e,o}$. We write

$$H = H_0 + H_{\text{barrier}}, \quad (11)$$

where $H_0 = \sum_{k>0} \hbar v_F k[\psi_e^\dagger \psi_e + \psi_o^\dagger \psi_o]$ is the kinetic energy expressed in the (e, o) basis, and $H_{\text{barrier}} = U(2k_F)(\psi_L^\dagger \psi_R + \psi_R^\dagger \psi_L) + U(0)(\psi_L^\dagger \psi_L + \psi_R^\dagger \psi_R)$ is the potential due to scattering off of the core hole (operators ψ_L and ψ_R are taken at $x = 0$). Expressed in terms of the bosonic operators, these may be written

$$H_0 = \frac{\hbar v_F}{8\pi} \int_{-\infty}^{\infty} d\tilde{x} \left\{[\nabla\phi_+(\tilde{x})]^2 + [\nabla\phi_-(\tilde{x})]^2\right\} \quad (12)$$

and

$$H_{\text{barrier}} = \frac{\hbar v_F}{2\pi} \left[\delta_+ \nabla\phi_+(\tilde{x}=0) + \delta_- \nabla\phi_-(\tilde{x}=0)\right], \quad (13)$$

where $\delta_\pm$ are related to $U(q)$ by Eq. (4), and we have defined $\phi_\pm = \phi_e \pm \phi_o$. Since this Hamiltonian is at most quadratic, it is a simple matter to compute the x-ray response exactly.

We now add an electron-electron interaction to the Hamiltonian (11), and in the long-wavelength limit write $H_{\text{int}} = V \int dx \rho_L(x)\rho_R(x)$, where the right and left moving electron densities are $\rho_{L,R}(x) = \psi_{L,R}^\dagger(x)\psi_{L,R}(x)$.[12] Expressed in terms of the boson fields, this takes the form

$$H_{\rm int} = V \int_{-\infty}^{\infty} d\tilde{x} \left[\frac{1}{16\pi^2} \tilde{\nabla}\phi_+(\tilde{x}) \tilde{\nabla}\phi_+(-\tilde{x}) - \frac{1}{4\pi^2\eta^2} \sin\phi_-(\tilde{x}) \sin\phi_-(-\tilde{x}) \right]. \quad (14)$$

Note that the Hamiltonian $H_0 + H_{\rm int} + H_{\rm barrier}$ decouples into independent ϕ_+ and ϕ_- channels. When $\delta_- = 0$, the effect of the barrier is contained only in the part dependent on ϕ_+, which is quadratic. Thus, as shown in Refs. 4 and 5, when $\delta_- = 0$ an exact solution is possible for arbitrary interaction strength. When δ_- is finite, the interaction term containing nonquadratic pieces makes a general solution difficult. Nonetheless, it is straightforward to expand perturbatively in $\gamma = V/2\pi\hbar v_F$, in order to show that δ_- changes drastically the x-ray-absorption edge singularity.

The x-ray response may be determined by computing $I(\epsilon) \propto {\rm Re} \int_0^\infty dt e^{i\epsilon t/\hbar} A(t)$ with

$$A(t) = \left\langle \psi_e(x=0,t) \exp\left\{ -\frac{i}{\hbar} \int_0^t H_{\rm barrier}(t')dt' \right\} \times \psi_e^\dagger(x=0,0) \right\rangle. \quad (15)$$

The averaging in Eq. (15) is performed over the ground state of the Hamiltonian $H_0 + H_{\rm int}$. To the lowest order in γ we find the correction to $I(\epsilon)$,

$$I(\epsilon) \propto \theta(\epsilon) \left(\frac{D}{\epsilon}\right)^{\alpha_0} \left[1 - \frac{\gamma}{4\pi} \left(\frac{\delta_-}{\pi} - 1 \right) \sin(2\delta_-) \ln^2 \frac{D}{\epsilon} \right] \quad (16)$$

with α_0 given by (3). For $\gamma = 0$ we recover the exact result for noninteracting electrons.[1,2,10] The first correction in γ diverges logarithmically as $\epsilon \to 0$.[12]

In logarithmic problems, a renormalization group analysis often allows one to extend the results of perturbation theory. Here we shall employ the usual program for the renormalization group. In (15) we thus divide $\phi_\pm$ into slow and fast components $\phi_\pm = \phi_\pm^< + \phi_\pm^>$, where $\phi^>$ is composed of Fourier components with $e^{-\ell}D < q < D$. Upon integrating out $\phi^>$ and rescaling space and time by a factor e^ℓ, we arrive at an equivalent problem with renormalized parameters. This procedure can easily be carried out perturbatively in γ, and we find that the lowest order renormalization group flow equation is

$$\frac{d\delta_-}{d\ell} = \frac{\gamma}{2} \sin 2\delta_-. \quad (17)$$

The related evolution of $A(t)$ is given by

$$\frac{d \ln A(t)}{d\ell} = -\frac{1}{2}\left(\frac{\delta_+}{\pi} - 1\right)^2 - \frac{1}{2}\left(\frac{\delta_-}{\pi} - 1\right)^2. \quad (18)$$

It may be observed that the perturbation theory result (16) satisfies this scaling relation. Equation (17) has been obtained earlier, in a study of the transmission coefficient of a barrier in a weakly interacting electron gas.[8] It shows that for an arbitrarily small backscattering, phase shifts will grow and at low energy scales phase shifts will saturate at $\pi/2$. For δ_- near 0 or $\pi/2$, Eq. (17) is equivalent to the weak interaction limit of the renormalization group flow equations derived for the weak and strong barrier limits in Ref. 7.

Equation (17) may simply be solved for the phase shift at any energy scale,

$$\delta_-(\ell) = \tan^{-1}[e^{\gamma\ell} \tan\delta_-(0)]. \quad (19)$$

We may obtain an expression for the correlation function $A(t)$ by integrating (18) down to an energy scale of order $De^{-\ell} \approx \hbar/t$,

$$A(t) = \exp\left[-\frac{1}{2}\left(\frac{\delta_+}{\pi} - 1\right)^2 \ln\frac{D_0 t}{\hbar} - \frac{1}{2}\int_0^{\ln Dt/\hbar} \left(\frac{\delta_-(\ell)}{\pi} - 1\right)^2 d\ell \right]. \quad (20)$$

In the weak interaction limit in which we are working, the Fourier transform of (20) may be found by noting that δ_- is a very slowly varying function of ℓ, so we obtain

$$I(\epsilon) \propto \left(\frac{D}{\epsilon}\right)^{-\frac{1}{2}\left(\frac{\delta_+}{\pi}-1\right)^2+1} \times \exp\left[-\frac{1}{2}\int_0^{\ln\frac{D}{\epsilon}} \left(\frac{\delta_-(\ell)}{\pi} - 1\right)^2 d\ell \right]. \quad (21)$$

Here $\delta_-(\ell)$ is given by Eq. (19). At relatively large energies, one should substitute into (21) the unrenormalized backscattering phase shift $\delta_-(0)$. If $\delta_-(0)$ is small, then $I(\epsilon)$ becomes a power law with the exponent (3). In the limit of small energies $\ell \to \infty$ the phase shift $\delta_- = \pi/2$, and (21) reduces to a power-law singularity with an exponent given by Eq. (7). As it follows from Eqs. (19) and (21) there is a clear crossover between these two regimes, if the initial value of phase δ_- is small. The crossover occurs at energy $\epsilon^* \sim D_0[\delta_-(0)]^{1/\gamma}$, in accordance with (8).

Since the Hamiltonian (14) is decoupled into independent + and − channels, it is clear that the Fermi-edge exponent should be the sum of two independent terms determined by δ_+ and δ_-, even when the interactions are not weak. The δ_+ term was computed in Refs. 4 and 5. Our solution of this problem in the weak interaction limit gives us strong indication of how the other term behaves in the intermediate interaction regime. In this regime, it is known that in a Luttinger liquid with repulsive interactions the renormalized backscattering grows as $U(2k_F) \propto (D_0/\epsilon)^{1-g}$, where $g = (1+2\gamma)^{-1/2}$.[7] Hence there is a crossover between the limits of weak and strong backscattering that occurs at $\epsilon^* \sim D_0[U(2k_F)/\hbar v_F]^{1/(1-g)}$. Recently, Prokof'ev[13] has computed the edge exponent at the strong backscattering fixed point ($\epsilon \to 0$). His result agrees with ours in the weak interaction limit. This is compelling evidence that the crossover physics described in Fig. 1 remains valid in the intermediate interaction regime (see also Ref. 14).

So far we considered the model of spinless electrons. An advantage of the perturbation theory in γ used here is that it allows a straightforward generalization to the case of spin-$\frac{1}{2}$ electrons. The energy dependence of the transmission coefficient (6), and consequently δ_-, is modified.[8] However the qualitative picture of the x-ray response behavior remains the same. As in the spinless case, δ_- renormalizes from its initial value to $\pi/2$, which leads to a crossover of the power-law exponent α. The limiting values of α may be found from Eq. (2). At large energies it gives $\alpha = (\delta_+ + \delta_-)/\pi - (\delta_+^2 + \delta_-^2)/\pi^2$, while near the threshold one obtains $\alpha = 1/4 + \delta_+/\pi - \delta_+^2/\pi^2$.

In conclusion, we studied the x-ray edge singularity for the weakly interacting 1D electron gas. We have shown that even a weak backscattering on the core hole affects this singularity drastically. It leads to the crossover in the dependence of the absorption-edge exponent on energy, as shown in Fig. 1. In the case of a weak core-hole potential, the x-ray exponent near the threshold equals 3/8 for spinless fermions and 1/4 for spin-$\frac{1}{2}$ electrons.

The authors are grateful to A. O. Gogolin for providing a copy of Ref. 14 prior to publication. C.L.K. acknowledges the hospitality of the Theoretical Physics Institute at the University of Minnesota where this work was started. K.A.M and L.I.G. acknowledge the hospitality of Aspen Center of Physics. This work was supported by the NSF Grant No. DMR-9117341.

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