X-ray-photoemission spectra of impure simple metals

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In this paper we study the influence of disorder on the x-ray-photoemission spectra of simple metals using functional methods. The exact long-time behavior of the core-hole Green's function is recovered for pure metals. The generalization to the case of impure metals yields an unusual time dependence for the core-hole Green's function. In the Drude region, the x-ray exponent is modified. Universal behavior is predicted close to the disorder-induced metal-insulator transition. Logarithmic relaxation occurs due to Mott's hopping conduction in the insulating region.

In theoretical investigation of the x-ray spectra of simple metals by Mahan,[1] an edge singularity in the absorption spectra was predicted due to the formation of excitons. It was pointed out by Anderson[2] that in addition to the excitonic effect the orthogonality catastrophe plays an important role. Both effects contribute to the low-frequency ($\omega \ll E_F$) power-law singularity of the core-hole–conduction electron correlation function, which is observed in absorption spectra of simple metals.[3] However, the absorption edge singularity could be annihilated due to the exciton mechanism.[1] On the other hand, photoemission spectra involve only the localized core-hole Green's function[4] where only the orthogonality catastrophe contributes. We will confine ourselves to the study of x-ray-photoemission spectra in this paper, since we are interested in the effect of disorder on the orthogonality catastrophe.

To the best of our knowledge this more realistic problem has not been addressed due to the difficulties involved in tackling disorder and interaction at the same time. The original diagrammatic formulation[5] is not easily adaptable to include disorder. In this paper we present a functional integral treatment of the problem which reproduces the known results and is readily extended to the case of disordered conductors.

This paper is organized as follows: In the first part we show that the core-hole Green's function can be expressed as a ratio of two Fredholm determinants and is evaluated in the long-time limit ($E_F t \gg 1$). It is seen that the long-time behavior is determined by the coupling of the core hole to the density fluctuations of the conduction electrons. The effect of disorder is studied in the second part. The expression in terms of determinants still holds; however, impurity averaging is required to obtain the Green's function. The long-time limit of the core-hole Green's function is studied in the diffusive, localized, and the Anderson transition regions. Universal time dependence of the core-hole Green's function close to the metal-insulator transition is predicted. It is suggested that this could be used experimentally as a signature of the localization transition. In the standard formulation[4,5] of the x-ray problem, one has the following imaginary-time action describing the interaction between the core hole $(d,\bar{d})$ and the conduction electrons $(c,\bar{c})$:

$$S[c,\bar{c};d\bar{d}]\equiv\int d^dx\int_0^\beta d\tau\,\bar{c}_x\left[\partial_\tau-\frac{\Delta}{2m}-\mu\right]c_x + \int_0^\beta d\tau\,\bar{d}(\partial_\tau-\varepsilon_d)d+V\int_0^\beta d\tau\,\bar{d}d\;\bar{c}_0c_0\;, \tag{1}$$

where μ is the chemical potential, $\beta=1/T$, V is the Coulomb energy, and $\hbar=1$. The core level ε_d is taken to be well below the conduction band so that overlap is negligible. For the present purpose of studying the effect of disorder on interaction we take the simplest model where the spin degrees of freedom and the momentum dependence of V are neglected (another way to think about this is to assume that the Coulomb interaction becomes short ranged due to screening).

The photoemission cross section is the Fourier transform of the core-hole Green's function.[1,4,5] The imaginary-time Green's function is defined as

$$\mathcal{G}_d(\tau_1,\tau_2)=-\langle d(\tau_1)\bar{d}(\tau_2)\rangle\;, \tag{2}$$

with

$$\langle(\cdots)\rangle=\frac{\int\mathcal{D}[c,\bar{c},d,\bar{d}]e^{-S}(\cdots)}{\int\mathcal{D}[c,\bar{c},d,\bar{d}]e^{-S}}\;.$$

In calculating $\mathcal{G}_d$ we follow the procedure reported elsewhere:[6] By integrating out the core hole we arrive at

$$\mathcal{G}_d(\tau_1,\tau_2)=\frac{\int\mathcal{D}[c,\bar{c}]\exp\left[-\int\bar{c}(\partial_\tau-\Delta/2m-\mu)c\right]\frac{F[\rho]}{f[0]}\mathcal{G}_d(\tau_1,\tau_2;[\rho])}{\int\mathcal{D}[c,\bar{c}]\exp(-\int\bar{c}(\partial_\tau-\Delta/2m-\mu)c)\frac{F[\rho]}{F[0]}}\ , \tag{3}$$

$$\frac{F[\rho]}{F[0]}\equiv\frac{\det(\partial_\tau-\varepsilon_d+V\rho)}{\det(\partial_\tau-\varepsilon_d)}\ , \tag{3a}$$

where $\rho=\bar{c}_0(\tau)c_0(\tau)$ is the conduction electron density at the origin (the location of the heavy hole) and $\mathcal{G}_d(\tau_1,\tau_2;[\rho])$ satisfies

$$[\partial_{\tau_1}-\varepsilon_d+V\rho(\tau_1)]\mathcal{G}_d(\tau_1,\tau_2;[\rho])=-\delta(\tau_1-\tau_2)\ . \tag{4}$$

It is seen that $\mathcal{G}_d[\rho]$ describes the propagation of the core hole under the influence of ρ. A simple calculation gives

$$\mathcal{G}_d(\tau_1,\tau_2;[\rho])=\mathcal{G}_d^0(\tau_1-\tau_2)\exp\left[-V\int_0^\beta d\tau S(\tau;\tau_1,\tau_2)\rho(\tau)\right], \tag{5}$$

where $\mathcal{G}_d^0$ is the free Green's function satisfying

$$[\partial_\tau-\varepsilon_d]\mathcal{G}_d^0(\tau)=-\delta(\tau) \tag{5a}$$

and

$$\mathcal{S}(\tau;\tau_1,\tau_2)=\frac{1}{\beta}\sum_\omega\frac{e^{-i\omega(\tau-\tau_1)}-e^{-i\omega(\tau-\tau_2)}}{i\omega}\ . \tag{6}$$

In Eq. (6), $\omega=2n\pi/\beta$ is the boson Matsubara frequency. At $T=0$, by replacing the sum over the Matsubara frequency by an integral, $\mathcal{S}$ becomes a switch function over the interval $\tau_1-\tau_2$:

$$\mathcal{S}(\tau;\tau_1,\tau_2)=\tfrac{1}{2}[\mathrm{sgn}(\tau-\tau_1)-\mathrm{sgn}(\tau-\tau_2)]\ . \tag{6a}$$

The determinant in Eq. (3a) describes in general the recoil of the heavy hole on the conduction electrons and is usually difficult to calculate except in a perturbation expansion. However, in the present problem the recoil is unity since there is only one hole. Mathematically, this can be seen by evaluating the determinant directly using the solution of Eq. (4), given by Eq. (5), and from the fact that the occupation number for the heavy hole is identically zero. This statement is verified in the Appendix.

We may therefore disregard the determinant while integrating out the conduction electrons in Eq. (3);

$$\frac{\mathcal{G}_d(\tau)}{\mathcal{G}_d^0(\tau)}=\frac{\det\left[\partial_{\tau'}-\frac{\Delta'}{2m}-\mu+V\delta(x')\mathcal{S}(\tau';\tau)\right]}{\det\left[\partial_\tau-\frac{\Delta}{2m}-\mu\right]}\ , \tag{7}$$

which was derived by Nozières and De Dominicis[5] and also appeared earlier in the context of the scattering phase shift in Fermi systems.[7] According to Eq. (7), the propagator is expressed in terms of the response of the electron gas to the localized time-dependent perturbation and we have

$$\ln\left[\frac{\mathcal{G}_d(\tau)}{\mathcal{G}_d^0(\tau)}\right]=-\int_0^V d\lambda\,\mathrm{tr}\mathcal{S}\mathcal{G}_c(\lambda)\ . \tag{8}$$

Note that a similar expression has been found by Hänsch and Minnhagen.[8]

The conduction electron Green's function $\mathcal{G}_c$ satisfies

$$\left[\partial_{\tau_1}-\frac{\Delta_{x_1}}{2m}-\mu+\lambda\delta(x_1)\mathcal{S}(\tau_1;\tau)\right]\mathcal{G}_c(x_1,\tau_1;x_2,\tau_2;\lambda)=-\delta(x_1-x_2)\delta(\tau_1-\tau_2) \tag{9}$$

and

$$\mathrm{tr}(\mathcal{S}\mathcal{G}_c)=\int_0^\beta d\tau'\int d^dx\,\delta(x)\mathcal{S}(\tau';\tau)\times\mathcal{G}_c(x,\tau';x,\tau'+0;\lambda)\ . \tag{10}$$

By expanding $\mathcal{G}_c$ to first order in $\mathcal{S}$, the coupling of the core hole to the density fluctuations of the conduction electrons is made evident while the zeroth-order term simply shifts ε_d,

$$\mathcal{G}_d(\tau)=\mathcal{G}_d^0(\tau)e^{-Q(\tau)}\ , \tag{11}$$

where

$$Q(\tau)=V^2\frac{1}{\beta}\sum_\omega\frac{1-\cos(\omega\tau)}{\omega^2}\int\frac{d^dk}{(2\pi)^d}\chi(k,|\omega|)\ . \tag{12}$$

At low frequency ($\omega\ll v_Fk$), the density correlator of the Fermi gas is $\chi\sim(\pi/2)\mathcal{N}|\omega|/v_Fk$, where $\mathcal{N}$ is the density of states at the Fermi level. [We are in the Matsubara representation, hence the form $|\omega|$. In the real-frequency domain the retarded density response function is $\mathrm{Im}\chi^R(\omega,k)\simeq-(\pi/2)\mathcal{N}\omega/v_Fk$.] We find at $T=0$

$$Q(\tau)=\frac{\bar{V}^2}{2}\ln[1+(E_c\tau)^2]\ ,$$

thus recovering the exact long-time behavior $\mathcal{G}_d(\tau)\sim(E_c\tau)^{-\bar{V}^2}$, for $E_c\tau\gg1$, where $E_c\sim E_F$ is the bandwidth cutoff and $\bar{V}=V\mathcal{N}$. The spectral function of $G^R(\omega)$ is

$$\mathrm{Im}G^R(\omega)\sim\frac{\sin\left[\frac{\pi}{2}\bar{V}^2\right]}{\Gamma(\bar{V}^2)}\frac{1}{E_c}\left[\frac{E_c}{\omega-\varepsilon_d}\right]^{1-\bar{V}^2}\quad\omega\simeq\varepsilon_d\ .$$

It is seen here that the infrared divergence $[\ln^n(E_c\tau)]$ generated in a perturbation series in V is exponentiated by Eq. (11). The logarithmic behavior of $Q(\tau)$ is caused by the Landau damping of the Fermi gas. However, impurity scattering gives rise to diffusive transport which

will become important for sufficiently high impurity concentration. From these considerations, we expect that the long-time behavior of the core-hole Green's function in a disordered metal would depend on the impurity-averaged density-density correlation function. This will be shown below. We take the model of a disordered metal as that proposed by Edwards.[9] The impurities are represented as elastic scattering centers distributed at random in the system. At finite concentration (C_i), the potential (U) seen by the conduction electrons becomes a Gaussian random field with zero mean and uncorrelated variance,

$$\langle U\rangle_U=0, \quad \langle U(\mathbf{x})U(\mathbf{x}')\rangle_U=\bar{U}^2\delta(\mathbf{x}-\mathbf{x}')$$

where

$$\bar{U}^w=C_i\left[\int d^dx\ U(\mathbf{x})\right]^2,$$

$$\langle(\cdots)\rangle_U=\frac{\int\mathcal{D}U\,P[U](\cdots)}{\int\mathcal{D}U\,P[U]},$$

and

$$P[U]\propto\exp\left[-\frac{1}{2\bar{U}^2}\int U^2\right].$$

Including the impurities the action becomes

$$S[c,\bar{c};d,\bar{d},U]=S[c,\bar{c};d,\bar{d}]+\int d^dx\int_0^\beta d\tau\,U(x)\bar{c}_xc_x\ . \tag{13}$$

The core-hole Green's functions is

$$\frac{\bar{\mathcal{G}}_d(\tau)}{\mathcal{G}_d^0(\tau)}=\left\langle\exp\left[-\int_0^V d\lambda\,\mathrm{tr}\mathcal{S}\mathcal{G}_c(\lambda,[U])\right]\right\rangle_U, \tag{14}$$

where $\langle\ \rangle_U$ denotes the impurity average. $\mathcal{G}_c(\lambda,[U])$ satisfies

$$\left[\partial_{\tau_1}-\frac{\Delta_{x_1}}{2m}-\mu+U(x_1)+\lambda\delta(x_1)\mathcal{S}(\tau_1;\tau)\right]\times\mathcal{G}_c(x_1,\tau_1;x_2,\tau_2;\lambda,[U])=-\delta(x_1-x_2)\delta(\tau_1-\tau_2)\ . \tag{15}$$

It is clearly difficult to perform the impurity average exactly. From the insight gained in the discussion of the pure case, one learns that the low-frequency properties of the emission spectra are determined by the coupling of the core hole to the density fluctuations of the electronic background. It is to be expected that such a mechanism still holds in the impure case. A cumulant expansion—here with respect to the random potential—is known to be applicable to the case where there is only a single core hole[1] and reveals just this coupling:

$$\bar{\mathcal{G}}_d(\tau)=\mathcal{G}_d^0(\tau)e^{-\bar{Q}(\tau)}, \tag{16}$$

where

$$\bar{Q}(\tau)=V^2\frac{1}{\beta}\sum_\omega\frac{1-\cos(\omega\tau)}{\omega^2}\int\frac{d^dk}{(2\pi)^d}\bar{\chi}_d(k,|\omega|)\ . \tag{17}$$

In the presence of disorder the density correlation function $\bar{\chi}_d(k,|\omega|)$ acquires a diffusion pole structure at small frequencies and momenta,

$$\bar{\chi}_d(k,|\omega|)=\frac{\pi\mathcal{N}|\omega|}{|\omega|+D_d(|\omega|)k^2}\quad\text{for } |\omega|\tau_i\ll1,\ kl\ll1\ , \tag{18}$$

while for $1/\tau_i<\omega<E_c$ and $1/l<k<k_F$ the Landau damping form of χ is adopted. In Eq. (18) $\tau_i^{-1}=\pi\mathcal{N}C_i\bar{U}^2$ is the rate of elastic collisions, $l=v_F\tau_i$ is the mean free path, and $D_d(|\omega|)$ denotes the diffusion coefficient in d dimensions. Corresponding to the diffusive and Landau damping behavior, the momentum integral in Eq. (17) is split into two regions: $\bar{Q}=\bar{Q}_{kl<1}+\bar{Q}_{kl>1}$, displaying the contribution of both transport processes. Let us first consider the insulating side of the localization transition. Clearly, there is no contribution from the Landau damping mechanism, since $k_Fl<1$ in this case, and the form of $D_d(|\omega|)$ will play a crucial role in determining $\bar{Q}(\tau)$. There exist excellent reviews[10–12] on the theory of localization where the calculation of $D_d(|\omega|)$ is discussed in detail. According to the standard theory of localization, all states are localized in dimensions $d\le2$, while there is a transition in higher dimensions. In the localized region, the diffusion coefficient is

$$D_d(|\omega|)=|\omega|\xi^2+(l|\omega|)^2\tau_i\ln(i|\omega|\tau_i)^{-(d+1)}, \tag{19}$$

where ξ is the correlation length, which diverges at the mobility edge and the logarithmic part is due to the hopping mechanism of Mott and Davis.[13] In one dimension, D has been found exactly,[14]

$$D_1(|\omega|)=4\zeta(3)|\omega|l^2+4(l|\omega|)^2\tau_i\ln(i2|\omega|\tau_i)^{-2}\ . \tag{20}$$

To a first approximation, the logarithmic terms in Eqs. (19) and (20) can be neglected since we are interested in the long-time behavior ($t\gg\tau_i$) of $\bar{Q}(t)$. Therefore $\bar{\chi}$ has practically no frequency dependence. From Eqs. (17)–(20), one see that $\bar{Q}(t)$ is purely imaginary,

$$\bar{Q}(t)=i\frac{\bar{V}^2}{g_0}A_d(\xi/l)\frac{t}{\tau_i}\quad(\text{for } T=0), \tag{21}$$

where $g_0=\mathcal{N}D_dl^{d-2}$ is the dimensionless Drude conductance with $D_d=(1/d)v_F^2\tau_i$ and

$$A_d(x)=\frac{1}{x^d}\int_{|y|<x}\frac{d^dy}{(2\pi)^d}\frac{1}{1+y^2}\ . \tag{22}$$

The frequency integral is evaluated with an exponential cutoff ($e^{-|\omega|\tau_i}$). The momentum integral is cut off at l^{-1}. From Eq. (21), one finds universal time dependence of $\bar{Q}(t)$ close to the localization transition. Although there is no gap in the electronic spectrum, the core-hole Green's function closely resembles that of an insulator. However, we find two important differences: (1) While the core level remains sharp there is a significant shift of ε_d,

$$\bar{\varepsilon}_d=\varepsilon_d+\frac{1}{\tau_i}\frac{\bar{V}^2}{g_0}A_d(\xi/l)\ . \tag{23}$$

(2) It was shown by Mott that there is hopping conductivity at finite frequency. By including the logarithmic terms from Eqs. (19) and (20), we find a slow-relaxation correction to $\bar{Q}(t)$,

$$\delta\bar{Q}_d(t)=\frac{\bar{V}^2}{g_0}B_d(\xi/l)f^d(t/\tau_i)\ , \tag{24}$$

where

$$f_d(t/\tau_i)=(-)^{d+1}\int_0^\infty\frac{dx}{x}[1-\cos(t/\tau_i)]\ln^{d+1}x\ e^{-x}$$
$$\sim\frac{1}{d+2}\ln^{d+2}\left[\frac{t}{\tau_i}\right]\quad(\text{for } t\gg\tau_i) \tag{25}$$

and

$$B_d(x)=\frac{1}{x^{d+2}}\int_{|y|<x}\frac{d^dy}{(2\pi)^d}\frac{y^2}{(1+y^2)^2}\ . \tag{26}$$

In one dimension, we have

$$\bar{Q}_1(t)=i\frac{\tan^{-1}[\zeta^{1/2}(3)]}{2\pi\zeta^{1/2}(3)}\frac{\bar{V}^2}{g_0}(t/\tau_i) \tag{27}$$

and

$$\delta\bar{Q}_1(t)=\frac{1}{2\pi\zeta^{3/2}(3)}\left[\frac{1}{2}\tan^{-1}[2\zeta^{1/2}(3)]-\frac{\zeta^{1/2}(3)}{1+4\zeta(3)}\right]\frac{\bar{V}^2}{g_0}f_1(t/2\tau_i)\ . \tag{28}$$

In the Drude region, both diffusive and ballistic transport contribute, and one has

$$\bar{Q}(t)=\frac{\bar{V}^2}{2\pi^2g_0}\ln(it/\tau_i)+\bar{V}^2\left[1-\left[\frac{1}{k_Fl}\right]^{-2}\right]\times\ln(iE_ct)\ . \tag{29}$$

Landau damping takes over when $k_Fl\gg1$, the first term in Eq. (29) is negligible, and we recover the clean-limit x-ray exponent. In the diffusive region and for sufficiently long time ($t\gg\tau_i, t\gg1/E_c$) the two terms in Eq. (29) can be combined as

$$\bar{Q}(t)=(\alpha_1+\alpha_2)\ln(it/t_0)\ , \tag{30}$$

where $\alpha_1=\bar{V}^2/(2\pi^2g_0)$, $\alpha_2=\bar{V}^2[1-(k_Fl)^{-2}]$, and $t_0=(\tau_i^{\alpha_1}E_c^{-\alpha_2})^{1/(\alpha_1+\alpha_2)}$. This shows that in the diffusive regime ($d=3$) the power-law behavior of the edge singularity survives, which is to be expected because the electronic states are extended. However, the exponent as well as the characteristic time scale are modified according to Eq. (30). Having studied the behavior of $\bar{Q}(t)$ in the diffusive and localized regions, we now turn to the transition regime. On the metallic side the diffusion coefficient is

$$D_3(|\omega|)=D(0)+|\omega|\xi^2\ , \tag{31}$$

where $D(0)$ vanishes at the critical impurity concentration.[12,15] It is clear from Eq. (17) that in the long-time limit the switch function introduces a lower cutoff $(1/t)$ in the frequency integral, and one has with Eqs. (18) and (31)

$$\bar{Q}(t)=\frac{\bar{V}^2}{g_0}\frac{1}{2\pi^2}\frac{1}{(\xi/l)^2}\frac{\tau_{\rm eff}}{\tau_i}\ln\left[1+i\frac{t}{\tau_{\rm eff}}\right]\ . \tag{32}$$

$\tau_{\rm eff}=\xi^2/D(0)$ defines the characteristic time scale of the system. Figure 1 shows the core-hole spectral function for $\bar{V}^2=0.5$. As $\tau_{\rm eff}$ diverges close to the transition, we may expand the logarithm in Eq. (32) and get

$$\bar{Q}(t)=i\frac{\bar{V}^2}{g_0}\frac{1}{2\pi^2}(l/\xi)^2t/\tau_i\ , \tag{33}$$

thus displaying universal long-time behavior. Note that Eq. (32) provides an interpolation between the insulating and the Drude regions: on the localized side it matches Eq. (21) for $\xi\gg l$, while on the metallic side, in the diffusive region, $D(0)/\xi^2\to1/\tau_i$, and the diffusive contribution to $\bar{Q}$ [Eq. (29)] is recovered. For sufficiently long time and at fixed $\tau_{\rm eff}$, we may identify an effective x-ray exponent from Eq. (32),

$$\bar{V}^2_{\rm eff}=\frac{\bar{V}^2}{g_0}\frac{1}{2\pi^2}\left[\frac{l}{\xi}\right]^2\frac{\tau_{\rm eff}}{\tau_i}\ , \tag{34}$$

which diverges $\sim1/D(0)$ as the localization transition is approached from the metallic side. However, the characteristic time $\tau_{\rm eff}$ (Refs. 11, 12, and 15) has an even stronger divergence. This implies a *sharpening* of the core-hole spectral function at the transition. This could be observed in experiments, since other structures in the spectral function are usually smeared out by disorder. Figure 2 shows the shift of the core level as a function of the disorder parameter W.

In this paper we have studied the effect of disorder on photoemission spectra. The picture that emerges is as follows: When an electron gas is suddenly perturbed its long-time response depends crucially on the way the

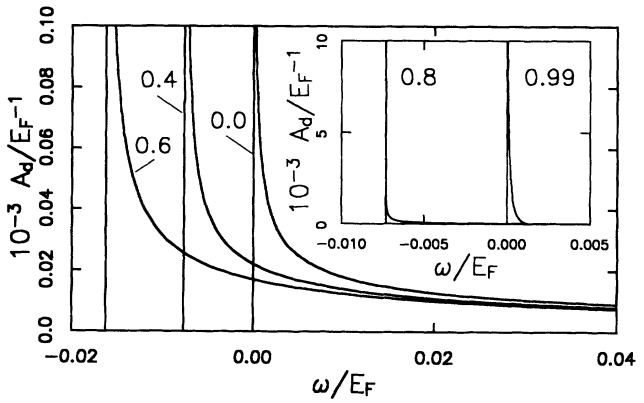

FIG. 1 Core-hole spectral function $A_d(\omega)$ for $\bar{V}^2=0.5$. The frequency is measured relative to the position of the clean x-ray singularity. Data for the parameters entering Eq. (32) were taken from a self-consistent diagrammatic theory of localization (Refs. 12 and 15), where a tight-binding model with rectangular distribution of impurities (width W) was adopted. A_d is shown for $W/W_c=0$, 0.4, 0.6, 0.8, and 0.99, with W_c the critical disorder.

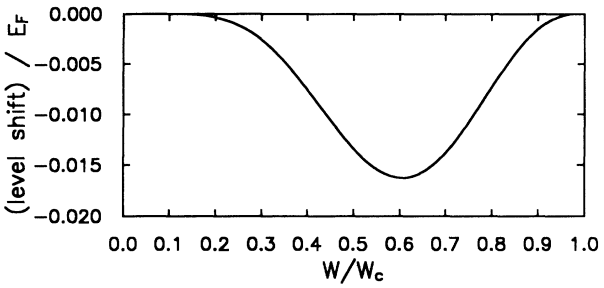

FIG. 2 Shift of the core level as a function of the disorder parameter W.

charges reorganize themselves.[2] Whenever there is finite charge transport either via diffusive or ballistic motion, the edge singularity in the photoemission spectra prevails. When charge transport ceases (i.e., in the insulating region) the edge singularity becomes a δ function centered at a renormalized core level. By including the Mott hopping mechanism at finite frequency, logarithmic relaxation is obtained, giving the spectral function a small spread. A formula is found which interpolates from the Drude regime up to the metal-insulator transition point. Between the clean and Drude limits an effective exponent is extracted which incorporates the two different types of charge transport. The collapse of the edge singularity into a δ-like peak at the transition could possibly be detected in x-ray photoemission experiments and shed light on the nature of the metal-insulator transition induced by disorder.

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APPENDIX: EVALUATION OF $F[\rho]\equiv\det(\partial_\tau-\varepsilon_d+V\rho)$

The quantity $F[\rho]$ has been calculated in many different ways in the literature. For the sake of completeness, we present here two more, the first of which is simple, because the nonperturbative solution Eq. (5) can be exploited to our advantage. The second method, which is based on perturbative expansion in ρ, requires a careful examination of a multiple phase-space integral, but gives the same conclusion.

Method I

Consider the ratio $F[\rho]/F[0]$. From the identity

$$\mathrm{tr}[\ln(A+B)]-\mathrm{tr}(\ln B)=\int_0^1 d\lambda\,\mathrm{tr}[B(A+\lambda B)^{-1}]\ , \tag{A1}$$

and identifying $A\equiv\partial_\tau-\varepsilon_d+V\rho$ and $B\equiv V\rho$, we find

$$-\ln\left[\frac{F[\rho]}{F[0]}\right]=\int_0^V d\lambda\,\mathrm{tr}(\rho\mathcal{G}_d[\rho])\ , \tag{A2}$$

where

$$\mathrm{tr}(\rho\mathcal{G}_d[\rho])=\int_0^\beta d\tau\,\rho(\tau)\mathcal{G}_d(\tau,\tau+0;\lambda[\rho])\ . \tag{A3}$$

But from Eq. (5) in the text,

$$\mathcal{G}_d(\tau,\tau+0;[\rho])=\mathcal{G}_d^0(\tau,\tau+0)\ , \tag{A4}$$

where

$$\mathcal{G}_d^0(\tau_1,\tau_2)=-\langle T_\tau d(\tau_1)\bar{d}(\tau_2)\rangle_0$$

is governed by the *free* Hamiltonian $H^0=\varepsilon_d d^\dagger d$. An elementary calculation gives

$$\begin{aligned}\mathcal{G}_d^0(\tau_{12})&=-\Theta(\tau_{12})e^{\varepsilon_d\tau_{12}}\langle dd^\dagger\rangle_0+\Theta(\tau_{21})e^{-\varepsilon_d\tau_{21}}\langle d^\dagger d\rangle_0\\&=-\Theta(\tau_{12})e^{\varepsilon_d\tau_{12}}\ ,\end{aligned} \tag{A5}$$

with $\tau_{12}\equiv\tau_1-\tau_2$, since we have a one-particle problem; $\langle d^\dagger d\rangle_0=0$ and from the anticommutator $[d,d^\dagger]_-=1$, $\langle dd^\dagger\rangle_0=1$. Hence $F[\rho]=F[0]$.

Method II

The perturbative expansion of the right-hand side of Eq. (A2) is

$$\begin{aligned}\int_0^V d\lambda\,\mathrm{tr}(\rho\mathcal{G}_d[\rho])&=V\int_0^\beta d\tau\,\rho(\tau)\mathcal{G}_d^0(\tau,\tau+0)\\&+\sum_{n=2}^\infty\frac{V^n}{n}\int_0^\beta d\tau_1\cdots\int_0^\beta d\tau_n\rho(\tau_1)\cdots\rho(\tau_n)\mathcal{G}_d^0(\tau_1-\tau_2)\cdots\mathcal{G}_d^0(\tau_{n-1}-\tau_n)\mathcal{G}_d^0(\tau_n-\tau_1)\ .\end{aligned} \tag{A6}$$

The first term in Eq. (A6) is clearly zero. We shall show that the remaining series vanishes *term by term*. Consider the $n=2$ case; we have typically

$$\int_0^\beta d\tau_1\int_0^\beta d\tau_2\cdots\Theta(\tau_{12})\Theta(\tau_{21})\ ,$$

from the fact the free Green's function is *purely* retarded. The product of step functions therefore puts a severe restriction in the domain of integration, which in this case is $(\tau_2>\tau_1)\cap(\tau_1>\tau_2)$, of measure zero. Next, consider $n=3$; the multiple integral becomes

$$\int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \int_0^\beta d\tau_3 \cdots \Theta(\tau_{12})\Theta(\tau_{23})\Theta(\tau_{31}) ,$$

where the domain of integration is $(\tau_2 > \tau_3 > \tau_1) \cap (\tau_1 > \tau_2 > \tau_3) \cap (\tau_3 > \tau_1 > \tau_2)$, again of measure zero. This process can be inductively generalized to all positive integers, implying the right-hand side of Eq. (A6) vanishes term by term. Indeed, the fact that $F[\rho] = F[0]$ is physically obvious; a one-particle sub system cannot have any influence on the vacuum. For the action given by Eq. (1) in the text the "no-recoil" approximation has already been built in, which is the physical mechanism that allows the x-ray problem to be trivially reduced to an equivalent one-body problem.

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