Density of states and screening near the mobility threshold

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The Hartree-Fock corrections to the density of states and to the thermodynamic quantities near the mobility threshold, necessitated by the interaction between the electrons, are calculated within the framework of the formalism of exact eigenfunctions. Principal attention is paid to the region of localized states. The "localization" corrections directly connected with the electron-return probability are found. Using a self-consistent localization theory, the known results of Aronov and Al'tshuler are generalized to include the case of an insulator. The localization contribution to the polarization operator, corresponding to a non-ergodic behavior of the system and leading to a difference between the isothermal and adiabatic resposes, is considered. It is shown that the static isothermal dielectric constant has a metallic behavior and corresponds to a finite screening radius also in the dielectric "phase," whereas both the high-frequency and the adiabatic responses are described by expressions that are typical for dielectrics.

1. INTRODUCTION

In the theoretical study of electron localization in disordered systems, which is attracting so much attention of late, interelectron-interaction effects are usually disregarded.[1] Yet it is known that an important role is played by these effects both in metals with small impurity density,[2,3] and for electrons in strongly localized states.[4,5] In a number of recent approaches[6–11] to metal–insulator transitions in disordered systems attempts are made to take the influence of interelectron interaction into account. All these studies deal only with the metallic (or quasimetallic in the case of two-dimensional systems) "phase" in the vicinity of the Anderson (or Mott) transition, and the insulator phase is disregarded. The role of interelectron interactions for localized electrons was considered, besides the already mentioned Refs. 4 and 5, only in various attempts to develop a theory for Fermi glasses.[12,13] All these studies demonstrate the important, if not decisive, role of correlations in the description of metal–insulator transitions in disordered systems. At the same time, the results of these studies are highly contradictory and the problem is still far from completely solved. There is even no clear answer to such a fundamental question as the possible existence of localization itself in systems with interaction. The situation is aggravated by the known difficulties[1] that arise in the theoretical description of the Anderson transition even in the one-electron application.

This being the situation, it makes sense to analyze first the case of weak interaction for strong disorder, as an attempt to determine which physical processes are particularly strongly influenced by the correlation. The present paper is devoted to the first-order perturbation-theory corrections to the density of states and to certain other characteristics of the system in the vicinity of the Anderson transition; principal attention will be paid to the region of localized state. In this sense, an attempt is made here to extend and generalize the known results of Aronov and Al'tshuler[2] for the metallic phase to include also the insulator state. We shall employ mainly the method proposed in Ref. 14 to derive the main results of Ref. 2. We shall regard the Anderson single-electron problem as solved, and for many actual calculations we shall use the self-consistent localization theory in the variant proposed by Vollhardt and Wölfle,[1] which comprises apparently a qualitatively correct interpolation analysis scheme that permits a description of the entire region of the transition from a metallic into a localized phase.[16–18]

2. GENERAL RELATIONS

Regarding the single-electron problem as solved, we introduce a complete orthonormalized system of exact wave functions $\varphi_\nu(\mathbf{r})$ and the corresponding eigenvalues of the electron energy in the random field of a disordered system. These functions and energies can correspond to both localized and delocalized states. We consider the single-electron causal Green's function in the representation of these exact eigenfuctions, particularly its diagonal matrix element

$$G_{\nu\nu}(\varepsilon)=\langle\nu|(\varepsilon-H+i\delta\operatorname{sign}\varepsilon)^{-1}|\nu\rangle, \tag{1}$$

where H is the total Hamiltonian that takes the interelectron interaction into account and ε is the energy reckoned from the Fermi level. The influence of the interaction is taken into account by introducing a corresponding self-energy part $\Sigma_\nu(\varepsilon)$ (Refs. 12–14).

$$G_{\nu\nu}(\varepsilon)=[\varepsilon-\varepsilon_\nu-\Sigma_\nu(\varepsilon)]^{-1},\quad \Sigma_\nu(\varepsilon)=\Delta_\nu(\varepsilon)+i\Gamma_\nu(\varepsilon)\operatorname{sign}\varepsilon. \tag{2}$$

Following the standard procedure[14,19] we introduced the renormalized energy $\tilde{\varepsilon}_\nu$ as the solution of the equation

$$\tilde{\varepsilon}_\nu-\varepsilon_\nu-\Delta_\nu(\tilde{\varepsilon}_\nu)=0, \tag{3}$$

and represent (2) at $\varepsilon\approx\tilde{\varepsilon}_\nu$ in the form

$$G_{\nu\nu}(\varepsilon)=Z_\nu[\varepsilon-\tilde{\varepsilon}_\nu+i\gamma_\nu\operatorname{sign}\varepsilon]^{-1}, \tag{4}$$

where

$$Z_\nu=\left[1-\frac{\partial\Delta_\nu(\varepsilon)}{\partial\varepsilon}\right]^{-1}_{\varepsilon=\tilde{\varepsilon}_\nu},\quad \gamma_\nu=Z_\nu\Gamma_\nu(\varepsilon=\tilde{\varepsilon}_\nu). \tag{5}$$

We introduce 14 the self-energy part $\tilde{\Sigma}_E(\varepsilon)$ averaged over some equal-energy surface $E=\varepsilon_\nu$ and over the configuration of the disordered-system random field that defines

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the single-electron problem:

$$\Sigma_E(\varepsilon)=\tilde{\Delta}_E(\varepsilon)+i\Gamma_E(\varepsilon)=N_0^{-1}(E)\left\langle\sum_\nu\delta(E-\varepsilon_\nu)\Sigma_\nu(\varepsilon)\right\rangle, \tag{6}$$

where the angle brackets denote the aforementioned configuration averaging and $N_0(E)$ is the single-electron (averaged) density of states.

We shall be interested in the single-electron density of states with account taken of the interaction; we define this state in the usual fashion

$$N(E)=-\pi^{-1}\left\langle\sum_\nu \operatorname{Im} G_{\nu\nu}^R(E)\right\rangle. \tag{7}$$

Assuming the corrections for the interaction to be small, $\gamma_\nu \ll \varepsilon_\nu \sim \tilde{\varepsilon}_\nu$, it is easy to verify that in first-order approximation

$$\frac{\delta N(E)}{N_0(E)}\equiv\frac{N(E)-N_0(E)}{N_0(E)}\approx-\frac{\partial\tilde{\Delta}_E(\tilde{\varepsilon}_\nu)}{\partial E}+\frac{\partial\tilde{\Delta}_E(\tilde{\varepsilon}_\nu)}{\partial\tilde{\varepsilon}_\nu}. \tag{8}$$

For reasons explained below we shall call the quantity

$$\frac{\delta\tilde{N}(E)}{N_0(E)}=-\frac{\partial\tilde{\Delta}_E(\tilde{\varepsilon}_\nu)}{\partial E} \tag{9}$$

the correction to the thermodynamic density of states. This density of states was first introduced in Ref. 14 (see also Ref. 8).

3. CORRECTIONS FOR INTERACTION: CONTRIBUTION FROM LOCALIZATION

We shall consider hereafter a model problem in which the interelectron interaction is described by a static repelling potential with a finite effective radius:

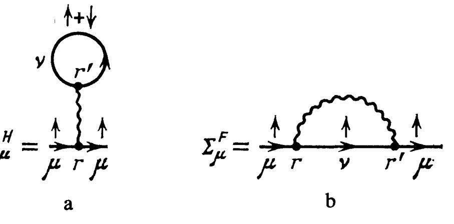
$$H_{int}=\frac{1}{2}\int d\mathbf{r}\int d\mathbf{r}'$$
$$\times\sum_{\mu\nu\mu'\nu'}\varphi_\mu^*(\mathbf{r}')\varphi_\nu^*(\mathbf{r})v(\mathbf{r}-\mathbf{r}')\varphi_{\mu'}(\mathbf{r})\varphi_{\nu'}(\mathbf{r}')a_\mu^+a_\nu^+a_{\mu'}a_{\nu'}. \tag{10}$$

An examination of the Hartree and Fock diagrams (Fig. 1) yields then

$$\Sigma_\mu^H=\int d\mathbf{r}\int d\mathbf{r}'\,v(\mathbf{r}-\mathbf{r}')\sum f_\nu\varphi_\mu^*(\mathbf{r}')\varphi_\nu^*(\mathbf{r})\varphi_\nu(\mathbf{r})\varphi_\mu(\mathbf{r}'),$$

$$\Sigma_\mu^F=-\int d\mathbf{r}\int d\mathbf{r}'\,v(\mathbf{r}-\mathbf{r}')\sum_\nu f_\nu\varphi_\mu^*(\mathbf{r}')\varphi_\nu^*(\mathbf{r})\varphi_\mu(\mathbf{r})\varphi_\nu(\mathbf{r}'), \tag{11}$$

where $f_\nu=f(\varepsilon_\nu)$ is the Fermi distribution function. We have accordingly from the definition (6)



a b

FIG. 1.

$$\tilde{\Sigma}_E^{H,F}=\int_{-\infty}^{\infty}d\omega\,f(E+\omega)\int d\mathbf{r}\int d\mathbf{r}'\,v(\mathbf{r}-\mathbf{r}')\langle\langle\rho_E(\mathbf{r})\rho_{E+\omega}(\mathbf{r}')\rangle\rangle^{H,F}, \tag{12}$$

where we have introduced the following spectral densities:

$$\langle\langle\rho_E(\mathbf{r})\rho_{E+\omega}(\mathbf{r}')\rangle\rangle^H=\frac{1}{N_0(E)}\left\langle\sum_{\mu\nu}\delta(E-\varepsilon_\mu)\delta(E+\omega-\varepsilon_\nu)\right.$$
$$\left.\times\varphi_\mu^*(\mathbf{r}')\varphi_\mu(\mathbf{r}')\varphi_\nu^*(\mathbf{r})\varphi_\nu(\mathbf{r})\right\rangle, \tag{13a}$$

$$\langle\langle\rho_E(\mathbf{r})\rho_{E+\omega}(\mathbf{r}')\rangle\rangle^F=\frac{1}{N_0(E)}\left\langle\sum_{\mu\nu}\delta(E-\varepsilon_\mu)\delta(E+\omega-\varepsilon_\nu)\right.$$
$$\left.\times\varphi_\mu^*(\mathbf{r}')\varphi_\mu(\mathbf{r})\varphi_\nu^*(\mathbf{r})\varphi_\nu(\mathbf{r}')\right\rangle. \tag{13b}$$

The spectral density (13b) was first considered by Berzinskiĭ and Gor'kov[20] in connection with a general localization criterion formulated in it. The gist of this criterion is that at energies $E<E_c$ (where E_c is the mobility threshold), i.e., in the region of the localized states, these spectral densities acquire a contribution that is a δ function of ω:

$$\langle\langle\rho_E(\mathbf{r})\rho_{E+\omega}(\mathbf{r}')\rangle\rangle^H=A_E(\mathbf{r}-\mathbf{r}')\delta(\omega)+\rho_E^H(\omega,\ \mathbf{r}-\mathbf{r}'), \tag{14a}$$

$$\langle\langle\rho_E(\mathbf{r})\rho_{E+\omega}(\mathbf{r}')\rangle\rangle^F=A_E(\mathbf{r}-\mathbf{r}')\delta(\omega)+\rho_E^F(\omega,\ \mathbf{r}-\mathbf{r}'), \tag{14b}$$

where the quantity

$$A_E(\mathbf{r}-\mathbf{r}')=\frac{1}{N_0(E)}\left\langle\sum_\mu\delta(E-\varepsilon_\mu)|\varphi_\mu(\mathbf{r})|^2|\varphi_\mu(\mathbf{r}')|^2\right\rangle$$
$$\neq 0,\quad E<E_c \tag{15}$$

is connected[21] with the probability of the electron returning to the initial point, so that the Berezinskiĭ–Gor'kov localization criterion is equivalent to the known Economou–Cohen criterion.[22] The validity of (14a) can be verified directly by repeating the arguments of Ref. 20.

Substituting (14) in (12) we obtain the following contributions to $\tilde{\Sigma}_E$, which is due to the onset of localized states in the system:

$$\tilde{\Sigma}_{E\,loc}^{H,F}=\tilde{\Delta}_{E\,loc}^{H,F}=\pm f(E)\int d\mathbf{r}\int d\mathbf{r}'v(\mathbf{r}-\mathbf{r}')A_E(\mathbf{r}-\mathbf{r}')$$
$$=\pm f(E)\int\frac{d^d\mathbf{q}}{(2\pi)^d}v(-\mathbf{q})A_E(\mathbf{q}), \tag{16}$$

where we have transformed in the last equation to the Fourier representation (d is the dimensionality of space). For a point interaction $v(\mathbf{r}-\mathbf{r}')=v_0\delta(\mathbf{r}-\mathbf{r}')$ we have

$$\tilde{\Sigma}_{E\,loc}^{H,F}=\pm f(E)v_0\int\frac{d^d\mathbf{q}}{(2\pi)^d}A_E(\mathbf{q})\equiv\pm f(E)v_0A_E, \tag{17}$$

where A_E is proportional[21] to the total probability of the electron returning to the initial point after an infinite time. We note that for a point interaction, by virtue of a property obvious from (13)

$$\langle\langle\rho_E(\mathbf{r})\rho_{E''}(\mathbf{r})\rangle\rangle^H=\langle\langle\rho_E(\mathbf{r})\rho_{E'}(\mathbf{r})\rangle\rangle^F \tag{18}$$

the "regular" contributions to $\tilde{\Sigma}_E^H$ and $\tilde{\Sigma}_E^F$ due to $\rho_E^{H,F}$ in (14) are equal (and of opposite sign).

For zero-spin fermions, the Hartree and the Fock contributions (17) cancel each other. It can be easily seen from (16) this cancellation does not depend on the interaction radius. When the spin is taken into account the Hartree contribution acquires an "extra" factor 2 connected with the summation over the spin in the electron loop of Fig. 1a. This results in a nonzero localization contribution:

$$\tilde{\Sigma}^{H+F}_{E\,loc}=\tilde{\Delta}^{H+F}_{E\,loc}=f(E)\,v_0A_E. \tag{19}$$

We write down for the sake of argument the equations for the point interaction. We recognize that the main energy dependence in (19) is determined by a Fermi function that varies strongly near the Fermi energy E_F. The quantity A_E at $E\approx E_F$ can be regarded as a constant (a smooth function of E). This assumption can, generally speaking, turn out to be correct near the mobility threshold, when A_E vanishes. The corresponding "critical exponent" is not known exactly, but it can be concluded from the available estimates[21] that $\partial A_E/\partial E\to 0$ also as $E\to E_c$. We then obtain from (9) and (19)

$$\left(\frac{\delta N(E)}{N_0(E)}\right)_{loc}=-\frac{\partial}{\partial E}\Delta^{H+F}_{E\,loc}\approx v_0A_{E_F}\left(-\frac{\partial f(E)}{\partial E}\right). \tag{20}$$

The singular (localization) contribution (20) is cancelled in the total density of states defined in (7) by the second term of (8):

$$\frac{\partial}{\partial\tilde{\varepsilon}_\nu}\tilde{\Delta}^{H+F}_{E\,loc}=\frac{1}{N_0(E)}\left\langle\sum_\nu\frac{\partial\Delta^{H+F}_\nu(\tilde{\varepsilon}_\nu)}{\partial\tilde{\varepsilon}_\nu}\delta(E-\tilde{\varepsilon}_\nu)\right\rangle$$

$$=\frac{1}{N_0(E)}\left\langle\sum_\nu\int d\mathbf{r}\int d\mathbf{r}'\right.$$

$$\left.\times v(\mathbf{r}-\mathbf{r}')\frac{\partial f_\nu}{\partial\varepsilon_\nu}\delta(E-\varepsilon_\nu)\,|\varphi_\nu(\mathbf{r})|^2|\varphi_\nu(\mathbf{r}')|^2\right\rangle=v_0A_{E_F}\frac{\partial f(E)}{\partial E}. \tag{21}$$

We shall see nevertheless that the thermodynamic density of states (9) governs the behavior of a number of thermodynamic quantities, and retains the localization contribution (20).

To understand better the physical meaning of the localization contribution to $\tilde{\Sigma}^{H+F}_E$, we note that in fact we are dealing here with allowance for the interaction of electrons that are in one and the same quantum state ν. It can be seen that in the case of diagrams *a* and *b* of Fig. 1 the contributions from the interaction of electrons with equal spin projections (shown by arrows in Fig. 1) cancel out completely, and $\tilde{\Delta}^{H+F}_{E\,\mathrm{loc}}$ is determined by the interaction of two electrons with opposite spins, which are in a state ν, i.e., by an effective interaction of the Hubbard type:

$$H_{eff}=\frac{1}{2}\sum_{\nu\sigma}\int d\mathbf{r}\int d\mathbf{r}'v(\mathbf{r}-\mathbf{r}')\,|\varphi_\nu(\mathbf{r})|^2|\varphi_\nu(\mathbf{r}')|^2n_{\nu\sigma}n_{\nu-\sigma}, \tag{22}$$

where $n_{\nu\sigma}$ is the operator of the number of electrons in a state ν and with a spin σ. Using the simplest estimate of A_E (Ref. 21) we have $(E_F<E_c)$

$$\tilde{\Delta}^{H+F}_{E\,loc}\approx\begin{cases}v_0R^{-d}_{loc}(E), & E<E_F\\ 0, & E>E_F\end{cases}, \tag{23}$$

where $R_{\mathrm{loc}}(E)$ is the localization radius of the electronic states with energy E. Comparing the results with Mott's known qualitative reasoning,[23] we see that $\tilde{\Delta}^{H+E}_{E_{loc}}$ coincides with the width of the narrow band of "singly occupied" electronic states produced below the Fermi level in the localization region.

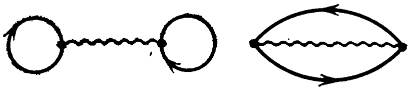


FIG. 2.

Considering the Hartree–Fock corrections to the thermodynamic potential, which are determined by the plots of Fig. 2, we obtain by direct calculation

$$\langle\delta\Omega_{H,F}\rangle=\int_{-\infty}^{\infty}dE\,f(E)N_0(E)\tilde{\Sigma}^{H+F}_E. \tag{24}$$

After integrating by parts we have

$$\delta\Omega=\langle\delta\Omega_H\rangle+\langle\delta\Omega_F\rangle=T\int_{-\infty}^{\infty}dE\,N_0(E)\left(\frac{\partial}{\partial E}\tilde{\Sigma}^{H+F}_E\right)\ln(1+e^{-E/T}). \tag{25}$$

Comparision of (25) and of the known expression for the thermodynamic potential of free fermions:

$$\Omega=-T\int_{-\infty}^{\infty}dE\,N(E)\ln(1+e^{-E/T}) \tag{26}$$

explains the use of the term "thermodynamic density of states" in connection with the definition (9). The singular (localization) part of the thermodynamic potential is given by

$$\delta\Omega_{loc}=\int d\mathbf{r}\int d\mathbf{r}'v(\mathbf{r}-\mathbf{r}')\int A_E(\mathbf{r}-\mathbf{r}')N_0(E)f^2(E)\,dE$$

$$=\int_{-\infty}dE\int\frac{d^d\mathbf{q}}{(2\pi)^d}v(-\mathbf{q})A_E(\mathbf{q})N_0(E)f^2(E). \tag{27}$$

The corresponding contributions to the entropy and to the heat capacity are

$$S_{loc}=-\frac{\partial\delta\Omega_{loc}}{\partial T}=-\int_{-\infty}^{\infty}dE\,N_0(E)\frac{\partial f^2(E)}{\partial T}v_0A_E\xrightarrow[T\to 0]{}v_0N_0(E_F)A_{E_F}, \tag{28}$$

$$C_{loc}=T\frac{\partial S_{loc}}{\partial T}\approx-\frac{\pi^2}{3}Tv_0\frac{\partial}{\partial E_F}\{N_0(E_F)A_{E_F}\}; \tag{29}$$

C_{loc} is connected with a small $(\sim\partial A_E/\partial E)$ correction to the thermodynamic potential. The corresponding correction to the density of states in (20) was neglected. The localization correction to the correlation contribution to the compressibility is also small:

$$\delta\varkappa_{loc}=-\frac{\partial^2}{\partial\mu^2}\delta\Omega_{loc}=-v_0\int_{-\infty}^{\infty}dE\,A_EN_0(E)\frac{\partial^2}{\partial\mu^2}f^2(E)$$

$$=v_0\frac{\partial}{\partial E_F}\{N_0(E_F)A_{E_F}\}. \tag{30}$$

Thus, the singular contribution (20) to the thermodynamic density of states does not lead to any contradiction whatever with the third law of thermodynamics. The finite contribution to the entropy as $T\to 0$ (28) is obviously due to the existence of "free" spins in the Mott strip.

4. REGULAR CONTRIBUTIONS

Up to now our analysis was quite general. We must now assume a certain specific one-electron model for the Anderson transition. We are principally interested in the contributions made to the density of states by the "regular" terms in the spectral densities (14). We confine ourselves only to the Fock contribution to (12) since, as noted in Refs. 3, 14, and 24, the Hartree contribution is small in terms of the parameter

$$F=\int d\Omega v\left(q=2p_F\sin\frac{\theta}{2}\right)\Big/\int d\Omega v(0), \tag{31}$$

where p_F is the Fermi momentum and the integration is over a solid angle on the Fermi surface. It is easily seen that $F<1$ if the interaction potential decreases over a length exceeding the reciprocal Fermi momentum. It can be verified[25] that the estimate (31) remains in force also for the regular contribution to (12) in the localized phase. For a point interaction, as is clear from (18), the Hartree contribution is double (when the spin is taken into account) the Fock contribution, so that the results that follow must simply be taken with the sign reversed.

As shown in Ref. 21, the connection between the Fourier transform of the spectral density (14b) and the two-particle Green's function of the one-electron problem is

$$\langle\langle\rho_E\rho_{E+\omega}\rangle\rangle_{\mathbf{q}}{}^F=\frac{1}{\pi N_0(E)}\operatorname{Im}\{\Phi^{RA}(E\omega\mathbf{q})-\Phi^{RR}(E\omega\mathbf{q})\}, \tag{32}$$

where

$$\Phi^{RA(R)}(E\omega\mathbf{q})=-\frac{1}{2\pi i}\sum_{\mathbf{pp}}\langle G^R(\mathbf{p}_+\mathbf{p}_+{}'E+\omega)G^{A(R)}(\mathbf{p}_-{}'\mathbf{p}_-E)\rangle,$$

$$\mathbf{p}_\pm=\mathbf{p}\pm\frac{\mathbf{q}}{2}. \tag{33}$$

A similar representation can also be written for (14a). At small ω and $\mathbf{q}$, the function $\Phi^{RR}(E\omega\mathbf{q})$, in contrast to $\Phi^{RA}(E\omega\mathbf{q})$, is regular.[15] We shall therefore neglect its contribution to the spectral density and assume it does not lead to a substantial renormalization of the density of states. As the one-electron model of the Anderson transition we employ the self-consistent localization theory in the form proposed by Vollhardt and Wölfle.[15–18] In this theory

$$\Phi^{RA}(E_F\omega\mathbf{q})=-N_0(E_F)[\omega+M_{E_F}(\mathbf{q}\omega)][\omega^2+\omega M_{E_F}(\mathbf{q}\omega)-2E_Fq^2/dm]^{-1}, \tag{34}$$

and the relaxation kernel M is determined as $q\to 0$ by the following self-consistent equation

$$M_{E_F}(\omega)=\frac{i}{\tau_0}\left\{1+\frac{1}{\pi N_0(E_F)}\int\frac{d^d\mathbf{q}}{(2\pi)^d}[-i\omega+D_{E_F}(\omega)q^2]^{-1}\right\}, \tag{35}$$

where

$$D_{E_F}(\omega)=\frac{2E_F}{dm}\frac{i}{M_{E_F}(\omega)} \tag{36}$$

is a generalized diffusion coefficient, τ_0 is the Born free-path time, and m is the electron mass. The solution of (35) is

$$M_{E_F}(\omega)=\frac{i}{\tau_{E_F}}-\frac{\omega_0{}^2(E_F)}{\omega}, \tag{37}$$

where

$$\omega_0{}^2(E_F)=-\lim_{\omega\to0}\omega M_{E_F}(\omega)>0$$

for $E_F<E_c$, i.e., below the mobility threshold whose location is defined by the equation $\omega_0^2(E_c)=0$. From (32) and (34) we easily obtain

$$\langle\langle\rho_E\rho_{E+\omega}\rangle\rangle_{\mathbf{q}}{}^F=\frac{1}{\pi}\frac{D_{E_F}q^2}{\omega^2+(D_{E_F}q^2)^2},\quad E_F>E_c,$$

$$\langle\langle\rho_E\rho_{E+\omega}\rangle\rangle_{\mathbf{q}}{}^F=A_{E_F}(q)\,\delta(\omega)+\frac{1}{\pi}\frac{D_{E_F}q^2}{\omega^2+[\omega_0{}^2(E_F)\tau_{E_F}+D_{E_F}q^2]^2}, \tag{38}$$

$E_F<E_c$,

where

$$A_{E_F}(q)=\frac{\omega_0{}^2(E_F)\tau_{E_F}}{\omega_0{}^2(E_F)\tau_{E_F}+D_{E_F}q^2}=(1+R^2_{loc}(E_F)q^2)^{-1}, \tag{39}$$

where $R^2_{\text{loc}}(E_F)=2E_F/dm\omega_0^2$ is the square of the localization radius and $D_{E_F}=(2E_F/dm)\tau_{E_F}$ is the renormalized diffusion coefficient. From (12) and (38) we obtain for the regular contribuiton $\tilde\Sigma_E^F$ at $T=0$:

$$\tilde\Sigma^F_{E\,reg}=-\frac{1}{\pi}\int_{-\infty}^{0}dE'\int\frac{d^d\mathbf{q}}{(2\pi)^d}v(\mathbf{q})\times\frac{D_{E_F}q^2}{(E'-E)^2+[\omega_0{}^2(E_F)\tau_{E_F}+D_{E_F}q^2]^2}. \tag{40}$$

For the correction to the density of states we obtain correspondingly

$$\frac{\delta N(E)}{N_0(E_F)}=-\frac{\partial}{\partial E}\tilde\Sigma^F_{E\,reg}=-\frac{1}{\pi}\int\frac{d^d\mathbf{q}}{(2\pi)^d}v(\mathbf{q})\frac{D_{E_F}q^2}{E^2+[\omega_0{}^2(E_F)\tau_{E_F}+D_{E_F}q^2]^2}. \tag{41}$$

Assuming now for simplicity the point-interaction model and recalling that up to now the energy E was reckoned from the Fermi energy E_F, we get for $2<d<4$

$$\frac{\delta N(E)}{N_0(E_F)}\approx\frac{v_0}{\pi}\frac{S_d}{d-2}D_{E_F}^{-d/2}=|E-E_F|^{(d-2)/2}-\tilde E^{(d-2)/2},$$

$$|E-E_F|\gg\omega_0{}^2(E_F)\tau_{E_F},$$

$$\frac{\delta N(E)}{N_0(E_F)}\approx\frac{v_0}{\pi}\frac{S_d}{d-2}D_{E_F}^{-d/2}=\omega_0^{d-2}(E_F)\tau_{E_F}^{(d-2)/2}-\tilde E^{(d-2)/2}, \tag{42}$$

$$|E-E_F|\ll\omega_0{}^2(E_F)\tau_{E_F},$$

where $S_d=[2^{d-1}\pi^{d/2}\Gamma(d/2)]^{-1}$. The characteristic energy E is connected here with the choice of the cutoff parameter on the upper limit of the integral with respect to q in (41). This cutoff is necessary because the "diffusion" approximation is not valid for the integrand and at large momenta. In accord with the consideration of the analogous cutoff in the integral of (35), which was carried out in Refs. 15 and 17, we choose a cutoff parameter equal to the Fermi momentum, so that

$$\tilde E=D_{E_F}p_F{}^2. \tag{43}$$

An alternative is the choice of a cutoff parameter equal to the reciprocal l^{-1} of the Born mean free path,[16] but near the mobility threshold we have $l^{-1}\sim p_F$, so that the two choices are equivalent. According to Lee's scaling reasoning,[8] near the mobility threshold, when $R_{\text{loc}}(E_F)\gg l, p_F^{-1}$, the cutoff parameter is proportional to R_{loc}^{-1} and $\tilde E\sim\omega_0^2(E_F)\tau_{E_F}$. This choice, however, contradicts the self-consistent localization theory on which our calculations are based. In fact, use of cutoff at momenta on the order of p_F or l^{-1} in the basic self-consistency equation (35) yields the usual results[15–17] that agree with the scaling picture of the Anderson transition.[15,16] On the other hand, using in (35) cutoff in the sense of Ref. 8 does not lead to equations in closed form. It must be emphasized, however, that in the self-consistent theory we still have the unsolved problem of determining the q dependence of the parameters $\omega_0^2(E_F)$ and D_{E_F} or τ_{E_F} at large q, since Eq. (35) is derived in the limit as $q \to 0$.

The estimate (50) is valid if the following condition

$$|E-E_F|,\ \omega_0^2(E_F)\tau_{E_F} \ll \tilde{E} \tag{44}$$

is satisfied. For the special case $d = 2$ we obtain in place of (42)

$$\frac{\delta N(E)}{N_0(E_F)} = \frac{v_0}{4\pi^2 D_{E_F}} \begin{cases} \ln \dfrac{|E-E_F|}{\tilde{E}}, & |E-E_F| \gg \omega_0^2(E_F)\tau_{E_F}, \\ \ln \dfrac{\omega_0^2(E_F)\tau_{E_F}}{\tilde{E}}, & |E-E_F| \ll \omega_0^2(E_F)\tau_{E_F}. \end{cases} \tag{45}$$

At $\omega_0^2(E_F) = 0$, i.e., in the metallic phase, Eqs. (42) and (44) agree with the usual results of Aronov and Al'tshuler.[2,3] It can be seen that at $|E - E_F| \gg \omega_0^2(E_F)\tau_{E_F}$ the metallic-phase kink in the density of the states at the Fermi level become smoothed out and is replaced by a smooth minimum. This conclusion, as can be easily verified, remains in force regardless of the cutoff used in the integral (41). A diagrammatic analysis in Ref. 25 has shown that (42) yields the main correction to the density of states everywhere except in an exponentially small vicinity of the Fermi surface, where an additional nonzero logarithmic contribution appears in the dielectric state.

We present actual relations that are obtained in the self-consistent localization theory. At $2 < d < 4$ and $E_F \lesssim E_c$ the solution of Eq. (35) produces in the dielectric phase (we omit some inessential constants)[17]

$$\omega_0^2(E_F) \sim E_F^2\left[1-\left(\frac{E_F}{E_c}\right)^{(4-d)/2}\right] \sim E_F^2\left|\frac{E_F-E_c}{E_c}\right|^{2/(d-2)}, \tag{46}$$

$$R_{loc}(E_F) \sim p_F^{-1}\left[1-\left(\frac{E_F}{E_c}\right)^{(4-d)/2}\right]^{-\nu} \sim p_F^{-1}\left|\frac{E_F-E_c}{E_c}\right|^{-\nu}, \tag{47}$$

$$\frac{\tau_{E_F}}{\tau_0} \sim \frac{d\lambda}{4-d}\left[\frac{d\omega_0^2(E_F)}{4E_F^2}\right]^{(d-2)/2} \sim \frac{d\lambda}{4-d}[p_F R_{loc}(E)]^{2-d} \sim \lambda\left|\frac{E_F-E_c}{E_c}\right|^{(d-2)\nu}, \tag{48}$$

where $\lambda = (2\pi E_F \tau_0)^{-1}$ is the dimensionless constant of perturbation theory in scattering by a disorder, and $\nu = (d-2)^{-1}$ is the critical exponent of the localization radius. The mobility threshold in the model of point scatterers randomly distributed in space at a density ρ and with a scattering amplitude V (Ref. 17) is

$$E_c \sim \left[\frac{{}'d}{d-2}(2\pi)^{-d/2}/\Gamma\left(\frac{d}{2}\right)\right]^{2/(4-d)} E_{sc},$$
$$E_{sc} = m^{d/(4-d)}(\rho V^2)^{2/(4-d)}. \tag{49}$$

Where E_{sc} is the "strong-coupling" energy.[1,2] At $E_F \sim E_{sc}$ we have $\lambda \sim 1$, and perturbation theory no longer holds. From (46)–(48) at $E_F \lesssim E_c$ we have

$$\omega_0^2(E_F)\tau_{E_F} \sim \frac{\lambda}{4-d}\frac{E_F}{[p_F R_{loc}(E_F)]^d} \sim \frac{\lambda E_F}{4-d}\left|\frac{E_F-E_c}{E_c}\right|^{d\nu}, \tag{50}$$

$$D_{E_F} \sim \frac{1}{4-d}\frac{1}{m}[p_F R_{loc}(E_F)]^{2-d} \sim \frac{1}{m}\left|\frac{E_F-E_c}{E_c}\right|^{(d-2)\nu}, \tag{51}$$

$$\tilde{E} \sim E_F[p_F R_{loc}(E_F)]^{2-d} \sim E_F\left|\frac{E_F-E_c}{E_c}\right|^{(d-2)\nu}. \tag{52}$$

It can be seen that satisfaction of the condition (44) entails no difficulty. For the correction to the density of states on the Fermi level ($|E - E_F| \ll \omega_0^2(E_F)\tau_{E_F}$) we obtain from (42) and (50)–(52) as $E_F \to E_c$

$$\frac{\delta N(E_F)}{N_0(E_F)} \sim \frac{4-d}{d-2} v_0 m^{d/2} E_F^{d/2-1}\{1-[p_F R_{loc}(E_F)]^{d-2}\} \sim -v_0 N_0(E_F)\left|\frac{E_F-E_c}{E_c}\right|^{-(d-2)\nu} \tag{53}$$

The divergence of the correction as $E_F \to E_c$, which follows from the last equality in (53) (a similar divergence occurs also in the metallic phase) indicates that our analysis cannot be used in the immediate vicinity of the mobility threshold. Our estimates are meaningful so long as $|\delta N(E)/N_0| \ll 1$. The divergence becomes logarithmic if the cutoff in (41) is in accord with the scheme of Ref. 8, in analogy with the corresponding result obtained there for the metallic region.

The corrections obtained above to the density of states can be found from the following qualitative arguments. Consider the interaction between an electron in a state ν with energy E, on the one hand, and an electron in a state with energy E_F, on the other. The relative correction to its wave function is then in first-order perturbation theory

$$\frac{\delta\varphi_\nu}{\varphi_\nu} \sim \int_0^\infty dt H_{int}(t), \tag{54}$$

where $t = 0$ is the instant when the interaction is turned on. After a time t the electron diffuses within the confines of the volume $(D_{E_F})^{d/2}$. We estimate the matrix element of the interaction for short-range repulsion at $v_0(D_{E_F}t)^{-d/2}$. Then

$$\frac{\delta\varphi_\nu}{\varphi_\nu} \sim v_0 \int_{t_{min}}^{t_{max}} dt (D_{E_F}t)^{-d/2} \sim v_0 D_{E_F}^{-d/2}\{t_{min}^{1-d/2} - t_{max}^{1-d/2}\}. \tag{55}$$

It is natural to determine $t_{\min}$ here from the condition for the applicability of the diffusion approximation: $(D_{E_F}t_{\min})^{1/2} \sim p^{F-1}$, i.e., $t_{\min} \sim (D_{E_F}p_F^2)^{-1} \sim \tilde{E}^{-1}$. The time $t_{\max}$ is determined by two factors. First, the matrix element of the interaction vanishes at times $t > |E - E_F|$ because of the of the temporal oscillations of the wave functions. Second, in the region of the localized states the interaction electrons cannot move apart by more than $R_{\text{loc}}(E_F)$, and the diffusion approximation is valid so long as

$t \lesssim R^2_{\mathrm{loc}}(E_F) D_{E_F} \sim (\omega_0^2 \tau_{E_F})^{-1}$. Therefore $t_{\max} \sim \min\{|E-E_F|^{-1}, (\omega_0^2\tau_{E_F})^{-1}\}$. Then, assuming that $\delta N(E)/N_0 \sim \delta\varphi_v/\varphi_v$, we obtain directly (42). Of course, these estimates are only purely explanatory.

The results provide a simple explanation of the analysis of Aronov and Al'tshuler[2,3] on the dielectric side of the Anderson transition. The approximations used do not contain a Coulomb gap,[4,5] primarily because of the short-range character of the interaction, and also perhaps because the model is crude and is based only on allowance for Hartree-Fock corrections.

5. POLARIZATION OPERATOR

We consider in this section, from a general viewpoint, how the localization affects the behavior of the polarization operator, i.e., actually the question of the character of the screening of the electric field in a Fermi glass.

Using again the representation of exact eigenfunctions of the one-electron problem, we have for the Fourier transform of the polarization operator of non-interacting electrons

$$\Pi(\mathbf{q}\omega) = \left\langle \sum_{\substack{\mu\nu\\ \mathbf{pp}'}} \frac{f_\mu - f_\nu}{\varepsilon_\mu - \varepsilon_\nu + \omega + i\delta\,\mathrm{sign}\,\omega} \times \varphi_\nu(\mathbf{p}_+)\varphi_\nu^*(\mathbf{p}_+')\varphi_\mu(\mathbf{p}_-')\varphi_\mu^*(\mathbf{p}_-) \right\rangle$$
$$= \int_{-\infty}^{\infty} dE \int_{-\infty}^{\infty} d\Omega \frac{f(E)-f(E+\Omega)}{\Omega+\omega+i\delta\,\mathrm{sign}\,\omega} N_0(E) \langle\langle \rho_E \rho_{E+\Omega} \rangle\rangle_{\mathbf{q}}^F \tag{56}$$

in the zero-temperature formalism and

$$\Pi(\mathbf{q}\omega_m) = \int_{-\infty}^{\infty} dE \int_{-\infty}^{\infty} d\Omega \frac{f(E)-f(E+\Omega)}{\Omega+i\omega} N_0(E) \langle\langle \rho_E \rho_{E+\Omega} \rangle\rangle_{\mathbf{q}}^E \tag{57}$$

in the Matsubara technique ($\omega_m = 2\pi m T$). Substituting the singular part of (14b) in (56), we obtain

$$\Pi_{loc}(\mathbf{q}\omega) = 0,$$

and a nonzero contribution comes only from the regular part of (14b):

$$\Pi(\mathbf{q}\omega) = \Pi_{reg}(\mathbf{q}\omega)$$
$$= \int_{-\infty}^{\infty} dE \int_{-\infty}^{\infty} d\Omega \frac{f(E)-f(E+\Omega)}{\Omega+\omega+i\delta\,\mathrm{sign}\,\omega} N_0(E) \rho_E^F(\mathbf{q}\Omega). \tag{58}$$

The situation in the Matsubara technique is different:

$$\Pi_{loc}(\mathbf{q}\omega_m \neq 0) = 0,$$
$$\Pi_{loc}(\mathbf{q}\omega_m = 0) = \int_{-\infty}^{\infty} dE \left(-\frac{\partial f(E)}{\partial E}\right) N_0(E) A_E(\mathbf{q}) = N_0(E_F) A_{E_F}(\mathbf{q}), \tag{59}$$

so that

$$\Pi(\mathbf{q}\omega_m) = \frac{\delta_{m0}}{T} \int_{-\infty}^{\infty} dE f(E)[1-f(E)] N_0(E) A_E(\mathbf{q})$$
$$+ \int_{-\infty}^{\infty} dE \int_{-\infty}^{\infty} d\Omega \frac{f(E)-f(E+\Omega)}{\Omega+i\omega_m} N_0(E) \rho_E^F(\mathbf{q}\Omega). \tag{60}$$

Taking into account the explicit form of the regular part of the spectral density, which arises in the self-consistent theory (38), we can obtain

$$\Pi(\mathbf{q}\omega) = \Pi_{reg}(\mathbf{q}\omega) = N_0(E_F) \frac{D_{E_F} q^2}{D_{E_F} q^2 + \omega_0^2(E_F)\tau_{E_F} - i\omega}. \tag{61}$$

In the metallic phase $\omega_0^2(E_F) = 0$, and (61) reduces to the known expression for the polarization operator of a "dirty" metal.[2,3,7] in the localization region, recognizing that $\omega_0^2(E_F)\tau_{E_F} = D_{E_F} R_{\mathrm{loc}}^{-2}$ we

$$\Pi_{reg}(\mathbf{q}0) = N_0(E_F) q^2 [q^2 + R_{loc}^{-2}(E_F)]^{-1}. \tag{62}$$

Analogous calculations yield for the Matsubara polarization operator

$$\Pi(\mathbf{q}\omega_m) = N_0(E_F) \left\{ A_{E_F}(q)\delta_{m0} + \frac{D_{E_F}(\omega_m) q^2}{\omega_m + D_{E_F}(\omega_m) q^2} \theta(\omega_m) + \frac{D_{E_F}(-\omega_m) q^2}{-\omega_m + D_{E_F}(-\omega_m) q^2} \theta(-\omega_m) \right\}, \tag{63}$$
$$\theta(\omega_m) = \begin{cases} 1, & m \geqslant 0 \\ 0, & m < 0' \end{cases}$$

where the generalized diffusion coefficient is

$$D_{E_F}(\omega_m) = \frac{2E_F}{dm} \frac{i}{M_{E_F}(\omega_m)}, \quad M_{E_F}(\omega_m) = \frac{i}{\tau_{E_F}} - \frac{\omega_0^2(E_F)}{i\omega_m}. \tag{64}$$

The difference obtained in the behavior of the polarization operator at $T = 0$ and in the Matsubara technique, a difference that manifests itself only at zero frequency (screening of the static field), is the consequence of the known difference between the static adiabatic and static isothermal responses in systems with non-ergodic behavior.[26,27] The latter leads to the appearance of a δ-function anomaly of the spectral density at zero frequency, which in our case is a consequence of the Anderson localization—of a typically non-ergodic phenomenon. The Matsubara response "senses" the nonergodicity manifestation,[27] whereas the response determined by the commutator Green's functions is insensitive to it. The polarization operator is connected with the electronic compressibility. For the static isothermal compressibility we have (cf. Ref. 27)

$$\varkappa^T(\mathbf{q}0) = \Pi(\mathbf{q}\omega_m = 0), \tag{65}$$

whereas the adiabatic compressibility is

$$\varkappa^A(q0) = \Pi_{reg}(q\omega \to 0). \tag{66}$$

We get then from (58) and (59)

$$\varkappa^T(q0) - \varkappa^A(q0) = N_0(E_F) A_{E_F}(q) = N_0(E_F)[1 + q^2 R_{loc}^2(E_F)]^{-1}. \tag{67}$$

The fact that $A_{E_F}(q)$ determines the difference between the isothermal and adiabatic compressibilities was first noted in Refs. 28 and 29. This difference, naturally, appears only in the static response. From (59)–(62) we obtain for the static isothermal polarization operator

$$\Pi^T(q0) = \Pi(q\omega_m = 0) = \Pi_{loc}(q0) + \Pi_{reg}(q0)$$
$$= N_0(E_F) \left[\frac{1}{1 + q^2 R^2_{loc}(E_F)} + \frac{q^2}{q^2 + R^{-2}_{loc}(E_F)} \right] = N_0(E_F). \tag{68}$$

Accordingly, for the static adiabatic dielectric constant we have

$$\varepsilon^{A}(q\omega\to 0)=1+\frac{4\pi e^{2}}{q^{2}}\Pi_{reg}(q0)=\begin{cases}1+\varkappa_{D}^{2}/q^{2}, & q\geqslant R_{loc}^{-1}(E_{F}),\\ 1+\varkappa_{D}^{2}R_{loc}^{2}(E_{F}), & q\leqslant R_{loc}^{-1}(E_{F}),\end{cases}\qquad(69)$$

where $\varkappa_{D}^{2}=4\pi e^{2}N_{0}(E_{F})$, whereas the static isothermal dielectric constant is

$$\varepsilon^{T}(q0)=1+\frac{4\pi e^{2}}{q^{2}}\Pi^{T}(q0)=1+\frac{\varkappa_{D}^{2}}{q^{2}}.\qquad(70)$$

It is precisely the latter dielectric constant that agrees with a real experiment on the screening of a static external field.[30] It can be seen from (70) that the Fermi-glass screens a static field.[1)] This fact was first noted qualitatively in Refs. 30 and 31. At any arbitraily low temperture the hopping conduction over the localized states aligns the electrons in an Anderson dielectric in a way that ensures complete screening. The characteristic times are obviously determined here by the frequency $\omega^{*}\sim D_{\text{hop}}\,q^{2}$, where D_{hop} is the coefficient of diffusion due to the hopping conduction, and $q\sim 1/L$, where the length L is determined by the characteristic scale of the external-field inhomogeneities in the given experiment[30,31] (e.g., by the distance between the capacitor electrodes). It is precisely in the sense of the condition $\omega<\omega^{*}$ that one must understand the static character of the field (and of the response) in the formalism described above (in which hopping conduction is not taken explicitly into account).

The divergence of the dielectric constant, observed in the approach to the metal–insulator transition in the known experiments on P-doped Si (Ref. 32) is probably due to the divergence of the localization radius $R_{\text{loc}}(E_{F}\to E_{c})$ in (69). It would be quite interesting to attempt a measurement of the dielectric constant of this system in a static field.

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[1)] In the employed formalism it is possible also to demonstrate directly that the corrections to $\Pi(q_{0})$, which lead to singularities such as (42) in the density of states, are mutually cancelled out by the interaction. This agrees fully with the important circumstance noted in Refs. 8 and 9, viz., the screening radius is determined not by the density of state but by the quantity $\partial N/\partial\mu=\Pi(\mathbf{q}\to 0,0)$, where N is the total density of the electrons. This was not taken into account in Ref. 6.

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