Contents lists available at ScienceDirect

Solid State Communications

Communication

States-conserving density of states for Altshuler-Aronov effect: Heuristic derivation

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ARTICLE INFO

ABSTRACT

Altshuler and Aronov (AA) have shown that the electron-electron interaction in a weakly-disordered metal suppresses the single-particle density of states (DOS) in the vicinity of the Fermi level (E_F). According to the AA theory the suppressed DOS exhibits the energy dependence $\propto \sqrt{|E - E_F|}$ valid for $|E - E_F|$ smaller than a certain correlation energy U_{co}. Recent experiments have shown that at energies larger than U_{co} the DOS exhibits a states-conserving dependence on energy, namely, the states removed from near the Fermi level are found at energies above U_{co} in the energy range of about $3U_{co}$. In this work the AA effect is studied beyond the low energy limit theoretically. We consider the AA model in which the electrons interact via the statically screened Coulomb interaction and the modification of the DOS is due to the exchange part of the electron self-energy. We derive the states-conserving DOS heuristically. Namely, we show that the self-energy consists of a diverging part (which we skip on physical grounds) and of the small part of the order of the pair Coulomb energy. This small part gives the states-conserving DOS which is in qualitative accord with experimental observations at energies above U_{co} and which reproduces the AA result at energies below U_{co}.

1. Introduction

Altshuler and Aronov (AA) have shown [1–3] that the electron-electron (e-e) interaction in a weakly-disordered three-dimensional (3D) metal suppresses the single-particle density of states (DOS) in the vicinity of the Fermi level (E_F). Specifically, the AA theory predicts for the suppressed DOS the energy dependence $\propto \sqrt{|E - E_F|}$ which is valid for $|E - E_F| \lesssim U_{co}$ where U_{co} is a characteristic correlation energy. The DOS $\propto \sqrt{|E - E_F|}$ at energies $|E - E_F| \lesssim U_{co}$ was observed by tunneling spectroscopy [4–14] and by photoemission spectroscopy [15]. Some experiments [8–10,12,15] studied the DOS also for $|E - E_F| > U_{co}$. In particular, the aim of experiment [12] was to show that the DOS in presence of the AA effect exhibits a states-conserving dependence on energy. It has been found [12] that all states removed from near the Fermi level by the AA effect are found at energies above U_{co} in the energy range of 2–3 times U_{co}. However, the observed states-conserving DOS [12] was not compared with theory, because the relevant theories [1–3,16,17] studied the AA effect in the low energy limit. In this work we study the AA effect beyond the low energy limit theoretically. We consider the model [3, 17] in which the electrons interact via the statically screened Coulomb interaction and the modification of the DOS is due to the Fock part of the self-energy. We derive the states-conserving

DOS which is in qualitative accord with experimental observations at energies above U_{co} and which reproduces the AA theory at low energies. We show that, besides the direct experimental study of the states-conserving DOS [12], such DOS was present (but not noticed) also in other experiments [8–10].

In our model [3,17] electrons in the disordered metal interact via the static finite-ranged potential $V(\vec{r} - \vec{r}')$. If $V = 0$, the electrons interact only with the random potential $V_d(\vec{r})$, produced by disorder. In such case the electron energies E_m and wave functions φ_m obey the Schrodinger equation $H\varphi_m(\vec{r}) = E_m\varphi_m(\vec{r})$, where $H = -(\hbar^2/2\,\mathrm{m})\Delta_{\vec{r}} + V_d(\vec{r})$. If we treat the e-e interaction within the first order perturbation theory and consider only the Fock part of the interaction, E_m is modified to $\widetilde{E}_m$ as [17]

$$\widetilde{E}_m = E_m + \Sigma_m^x \tag{1}$$

where Σ_m^x is the Fock first-order self-energy correction:

$$\Sigma_m^x = -\sum_n f_n \int \frac{d\vec{q}}{(2\pi)^3}\, V(q)\left|\langle \varphi_m|e^{i\vec{q}\cdot\vec{r}}|\varphi_n\rangle\right|^2. \tag{2}$$

Here $V(q)$ is the Fourier transform of $V(\vec{r} - \vec{r}')$, f_n is the Fermi function, and Σ_n is the sum over n with spin parallel to that of m. Equations

(1) and (2) hold if $\Sigma_m^x \ll E_m$.

Equations (1) and (2) describe a specific disordered sample. When averaged over many disordered samples, they remain unchanged except that E_m and Σ_m^x are the mean values. Most important, the disorder-averaged $|\langle \varphi_m | e^{i\vec{q} \cdot \vec{r}} | \varphi_n \rangle|^2$ can be calculated explicitly. For a diffusing electron [3,16,17]

$$\left| \langle \varphi_m | e^{i\vec{q} \cdot \vec{r}} | \varphi_n \rangle \right|^2 = \frac{1}{\pi \rho(E_n) \Omega} \frac{\hbar D q^2}{(\hbar D q^2)^2 + (E_m - E_n)^2} \quad (3)$$

where D is the diffusion coefficient, Ω is the volume, and $\rho(E_n)$ is the DOS for a single spin orientation [$\rho(E_n)$ is often replaced by $\rho(E_F)$ which is justified for E_n close to E_F]. If we average $\widetilde{E}_m$, E_m, and Σ_m^x over all states m with energies $E_m = E$, equation (1) can be rewritten as

$$\widetilde{E}(E) = E + \Sigma^x(E) , \quad (4)$$

where

$$\Sigma^x(E) = - \int_0^{E_F} dE' \int \frac{d\vec{q}}{8\pi^4} V(q) \frac{\hbar D q^2}{(\hbar D q^2)^2 + (E - E')^2} . \quad (5)$$

In the last equation and in all following calculations we assume zero temperature for simplicity.

Due to averaging over disorder the unperturbed DOS (per spin) reads $\rho_0(E) = (m/2)^{3/2} \sqrt{E} / \pi^2 \hbar^3$, as for the free electrons. The perturbed DOS versus E, $dn/d\widetilde{E} \equiv \rho(E)$, can be expressed [3,16,17] from equation (4) as

$$\rho(E) = \rho_0(E) \frac{1}{1 + \frac{d\Sigma^x(E)}{dE}} \simeq \rho_0(E_F) \frac{1}{1 + \frac{d\Sigma^x(E)}{dE}}. \quad (6)$$

where the right hand side holds for $\rho_0(E) \simeq \rho_0(E_F)$. Note that the perturbed DOS, $\rho(E)$, is expressed as a function of E rather than of $\widetilde{E}$. This approximation is valid within the first order perturbation theory [3,16,17]

It is customary to change the integral $\int_0^{E_F} dE'$ in equation (5) as $\int_{-\infty}^{E_F} dE'$. This *infinite band* approximation is justified for weak interaction. Then, substituting E by variable $\varepsilon = E - E_F$, one can rewrite equation (5) as [16]

$$\Sigma^x(\varepsilon) = - \int_\varepsilon^\infty d\varepsilon' \frac{d\Sigma^x(\varepsilon')}{d\varepsilon'} , \quad (7)$$

where [3,16,17]

$$\frac{d\Sigma^x(\varepsilon)}{d\varepsilon} = \int \frac{d\vec{q}}{8\pi^4} V(q) \frac{\hbar D q^2}{(\hbar D q^2)^2 + \varepsilon^2} . \quad (8)$$

The AA effect was studied [3,16,17] for $V(q)$ so small that $d\Sigma^x(\varepsilon)/d\varepsilon \ll 1$. Then $\rho(E) \simeq \rho_0(E_F)[1 - d\Sigma^x(E)/dE]$, or

$$\rho(\varepsilon) \simeq \rho_0(0)[1 - d\Sigma^x(\varepsilon)/d\varepsilon]. \quad (9)$$

In the simplest model [3,16,17] with static screening

$$V(q) = \frac{e^2}{\varepsilon_\infty(q^2 + k_s^2)} , \quad (10)$$

where $k_s = \sqrt{e^2 2 \rho_0(E_F)/\varepsilon_\infty}$ is the reciprocal screening length (the factor of 2 is due to the spin degeneracy), and ε_∞ is the high-frequency permittivity of the metal.

From equations (8) and (9) one obtains the result of Altshuler and Aronov [1,17]

$$\rho(E) = \rho(E_F) + \frac{1}{4\sqrt{2}\pi^2} \frac{|\varepsilon|^{1/2}}{(\hbar D)^{3/2}}, \quad (11)$$

where $\rho(E_F)$ is the DOS at the Fermi level and the second term on the right hand side is the AA interaction correction. In Refs. [1,17] the integral in equation (8) was calculated assuming $V(q) \simeq V(0)$. For $V(q) = V(0)$ the integral diverges in the upper limit, therefore, the upper limit was restricted to $q_{max} = \sqrt{|\varepsilon|/\hbar D}$. Since $V(q) \simeq V(0)$ only for $q \lesssim k_s$,

the obtained result [equation (11)] holds only for $|\varepsilon| \lesssim \hbar D k_s^2$. Within this approach the term $\rho(E_F)$ remains undetermined, it is usually determined experimentally [14,15].
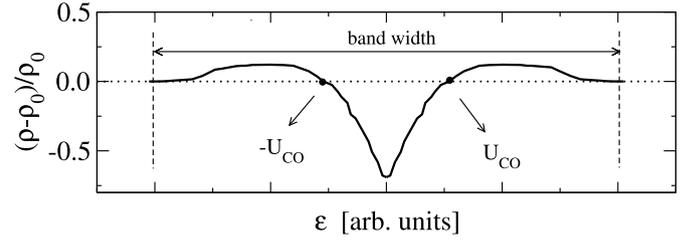
Fig. 1. Experimental output (schematic) for DOS in a weakly disordered metal, normalized as $[\rho(\varepsilon) - \rho_0(0)]/\rho_0(0)$. The correlation energy U_{co}, defined [12] by equation $\rho(\varepsilon) = \rho_0(0)$, is marked by arrow. The states conservation means that $\left| \int_0^{U_{co}} d\varepsilon (\rho - \rho_0)/\rho_0 \right| = \int_{U_{co}}^\infty d\varepsilon (\rho - \rho_0)/\rho_0$, assuming that the conduction band width is much larger than the states conservation region.

In the following text we present an alternative derivation which is not restricted to the low-energy limit. At low energies our derivation will reproduce equation (11) and also determine explicitly the term $\rho(E_F)$. However, our major goal is to go beyond the low energy limit and to derive the DOS which conserves the states similarly as in the experiment [12].

In Section 2 we show that the DOS given by equations 8–10 does not conserve the states. In Section 3. we identify why this is so and present a heuristic derivation of the states-conserving DOS. Comparison with experiment is presented in Sections 3 and 4. Finally, in Section 5 we interpret the AA effect with conservation of states in terms of coupling between the interaction (10) and matrix element (3).

2. The states conservation problem

Fig. 1 shows schematically the typical experimental output [12]. At energies below U_{co} the data show the AA singularity described by the $|\varepsilon|^{1/2}$ law. All states repelled from the AA singularity are found at energies above U_{co} in the range of about $3U_{co}$. This *local* conservation of states should be distinguished from the conservation of states in strongly correlated disordered systems where the states repelled by interaction are transferred far away from the Fermi level [18]. In the latter case one cannot use the approximation of the infinitely wide band which on the contrary has no effect if conservation of states takes place *locally* near the Fermi level. Whenever we speak about the conservation of states, we have in mind the *local* conservation of states similar to that in Fig. 1.

In accord with Fig. 1 and Ref. [12], the conservation of states for the AA model reviewed in Section 1 reads

$$\int_0^\infty d\varepsilon [\rho(\varepsilon) - \rho_0(0)] = 0 . \quad (12)$$

Inserting equation (9) into the conservation law (12) we find that the conservation of states is fulfilled only if

$$\int_0^\infty d\varepsilon \frac{d\Sigma^x(\varepsilon)}{d\varepsilon} = 0 . \quad (13)$$

However, equation (13) is not fulfilled because $d\Sigma^x(\varepsilon)/d\varepsilon$ is positive for any ε [see equation (8)]. This means that the model of Section 1 does not conserve the states.

Furthermore, integral $\int_0^\infty d\varepsilon\, d\Sigma^x(\varepsilon)/d\varepsilon$ not only fails to fulfill equation (13) but even diverges in the upper limit (see the next section). This means that also the self-energy (7) diverges which is another problem, in addition to the states conservation problem. In principle, the divergence could be eliminated by considering the energy band of finite width, however, the self-energy would then depend on the band