Local and total density of electronic states in metal-semimetal systems

L. B. Dubovskiĭ

I. V. Kurchatov Atomic Energy Institute

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A simple and convenient method is proposed for the analysis of the state density in sandwich structures, when the potential energy depends only on one coordinate. It is shown that in the general case the state density of the system can be broken up into three parts: 1) volume, uniformly built up over the entire volume of the system in proportion to the Fermi momentum at the corresponding point; 2) coherent, built up in proportion to the time of stay of the electron on a selected segment of a quasiclassical trajectory, with energy equal to the Fermi energy; 3) surface, built up over distances of the order of the wavelength near the surface. A detailed investigation is made of the situation wherein the coherence of the electron motion is violated in one part of the system (metal), while in another part (semimetal) the electron moves coherently. The conditions under which oscillations of the state density as functions of the semimetal thickness take place are made clear, and it is shown that the oscillating part of the state density builds up completely in the semimetal and attenuates outside the metal over distances of the order of the wavelength.

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I. INTRODUCTION

This paper is devoted to the electronic state density in sandwich structures of the metal–semimetal type. In these systems, the state density is highly inhomogeneous in space, and various measured quantities contain the state density not of the entire system but of its individual parts. Thus, the superconducting characteristics contain the state density of that region of space where pairing takes place. Therefore, in addition to the total state density, it is of interest to consider also the differential state density.

The article develops a convenient method for the analysis of the state density when, as in sandwich structures, the potential of the electrons depends on a single coordinate. We trace the accumulation of the total state density in different points of space. The total state density (see the group of papers by Balian and Bloch[1]) can be represented in the form of a sum of three terms. The first term g_V—volume—builds up uniformly in space and is proportional to the Fermi momentum k_F at the corresponding point of space:

$$g_V=\int\frac{d^3r}{4\pi^2}k_F(\mathbf{r}). \tag{1.1}$$

The two other terms have a scale $S/4\pi^2$, i.e., they are smaller by a factor $k_Fd\gg 1$ than g_V (S is the surface area of the sandwich and d is its linear dimension). The first, coherent term is the result of the motion of the electron over preferred (extremal) trajectories and oscillates as a function of the phase $\int k_F(l)dl$, built up over the entire trajectory of the electron. For the case of a sandwich, this means motion from one boundary of the sandwich to the other with zero transverse momentum. The coherent term g_{coh} builds up uniformly along the entire motion of the electron over the trajectory in proportion to the time of stay in the corresponding point of the trajectory or in inverse proportion to the particle momentum at this point.

The third term

$$g_S=\frac{1}{4\pi^2}\int d\sigma_S\left(\frac{\pi}{4}-\operatorname{arctg}\frac{\varkappa(S)}{k_F(S)}\right) \tag{1.2}$$

is connected with the motion of the electron near the boundary of the sandwich and builds up over a distance on the order of the wavelength of the electron near the corresponding boundary. We emphasize that in this case the electron wavelength $1/k_F(S)$ can be different in different sections of the system surface.

If coherence is violated in the course of motion of the electron from one surface to the other, then the coherent term g_{coh} in the state density yields zero after averaging, and we are left only with the two terms $-g_V$ and g_S [(1.1) and (1.2)]. Since only the coherent term, which builds up uniformly over the entire trajectory of the electron vanishes in scattering, it is immaterial whether the coherence is violated because of scattering in the volume of the system or because of scattering by the boundaries. All that matters is the very fact of violation of the coherence. The scattering in the system is simulated in this paper in two different ways: by averaging over the energy (see Ref. 1a) and by averaging of the results over the thickness of the system; this corresponds to the case when the system is inhomogeneous over its thickness.

The second of these methods of averaging makes it possible to treat more completely the situation formulated in the paper of Kagan and the author,[2] when the coherence of motion of the electron is violated only in part of the system, and in the other part of the system the electron moves without scattering. Namely: assume a metallic film on which a semimetallic coating is sputtered (see Fig. 1). We assume that the electron-motion coherence is violated in the metal of thickness d, but the motion of the electron is coherent in the semimetal of thickness t. This assumption is fully justified in

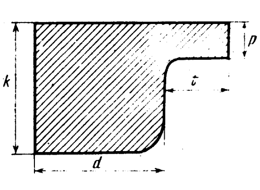

FIG. 1.

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many cases, since the electron wavelength is much smaller in the metal than in the semimetal, and the distortions experienced by the short-wavelength electrons in the metal are not felt by the long-wavelength electron in the semimetal (for details see Ref. 2).

This raises the question of identifying the quantities that are sensitive to the electron-motion coherence in the semimetal of thickness t. It turns out that the total state density of the system oscillates as a function of the semimetal thickness. These oscillations take place only if the potential on the metal–semimetal interface varies sufficiently rapidly, namely: the electron Fermi momentum in the transition layer must change by a value at least of the order of unity over a distance on the order of the wavelength. In real junctions this condition is actually always satisfied. In the opposite limiting case, when the Fermi momentum in the transition layer varies little over a distance on the order of the electron wavelength, the oscillations disappear. The period of the oscillations is $\int p(t)dt$ (the integration is over the semimetal, and $p(t)$ is the Fermi momentum in the semimetal). The oscillating part of the state density is built up uniformly over the entire semimetal–in inverse proportion to the Fermi momentum of the electron at each point of the semimetal, and attenuates over distances of the order of the wavelength in the metal near the metal–semimetal interface. At distances larger than the wavelength of the metal there are no state-density oscillations connected with the coherent motion in the semimetal.

II. LOCAL AND TOTAL STATE DENSITY IN AN ARBITRARY ONE-DIMENSIONAL POTENTIAL

The state density of the system is expressed in terms of an integral of imaginary part of the Green's function

$$g_\gamma(\mu) = -\frac{1}{\pi}\int_V d^3r[\operatorname{Im} G(\mathbf{r}\mathbf{r}', \mu+i\gamma)]_{\mathbf{r}'=\mathbf{r}}. \tag{2.1}$$

At $\gamma \to 0$, Eq. (2.1) represents the state density. At finite γ, the function $g_\gamma(\mu)$ is the Lorentz-averaged state density with width γ (see, e.g., Ref. 1a). The integration in (2.1) is over the entire volume of the system. We consider also the differential density of states, when the integration is only over the part of the system that is of interest. In a sandwich, the potential energy depends only on one coordinate, which we take to be x. In this case it is convenient to go over in (2.1) to the momentum representation in the coordinates y and z. As a result we obtain

$$g_\gamma(\mu) = -\frac{S}{2\pi^2}\int_0^\infty p_\perp\, dp_\perp \operatorname{Im} J_{tot}(p_\perp). \quad J_{tot}(p_\perp) = \int_0^d G_{p_\perp}(xx)\,dx. \tag{2.2}$$

The Green's function $G_{p_\perp}(xx')$ satisfies in this case the equation

$$d^2G(xx')/dx^2+[E-V(x)]G(xx') = \delta(x-x'), \qquad 0<x<d, \quad E=\mu-p_\perp^2+i\gamma. \tag{2.3}$$

We assume here for simplicity that $\hbar = 2m = 1$. We solve Eq. (2.3) subject to general boundary conditions of the form

$$\frac{dG}{dx}(0,x')-\varkappa_0 G(0,x')=0, \qquad \frac{dG}{dx}(d,x')+\varkappa_d G(d,x')=0. \tag{2.4}$$

To analyze Eq. (2.3) with boundary conditions (2.4), it is convenient to introduce the characteristic function $\varphi(x)$ satisfying the equation

$$d^2\varphi/dx^2+(E-V(x))\varphi(x)=0, \tag{2.5}$$

and also the conditions on the boundary:

$$\frac{d\varphi}{dx}(0)-\varkappa_0\varphi(0)=0, \qquad \varphi(0)=\frac{1}{\varkappa_0}. \tag{2.6}$$

For an arbitrary piecewise-constant potential, $\varphi(x)$ can be easily written out in general form, inasmuch as in this case (2.5) is an ordinary differential equation with constant coefficients. Besides the function $\varphi(x)$, we introduce also the function $\psi(x)$:

$$\psi(x)=\varphi(x)\int_x^d \frac{dx_1}{\varphi^2(x_1)}.$$

It is easy to verify directly that $\psi(x)$, just as the characteristic function $\varphi(x)$, satisfies Eq. (2.5). Furthermore, the functions $\varphi(x)$ and $\psi(x)$ are linearly independent solutions of Eq. (2.5), inasmuch as at all values of x we have

$$\varphi\frac{d\psi}{dx}-\psi\frac{d\varphi}{dx}=-1.$$

Therefore we can use $\varphi(x)$ and $\psi(x)$ to construct the function $G(xx')$:

$$G(xx')=\begin{cases}\varphi(x)[P\varphi(x')+R\psi(x')], & x<x'\\ [P\varphi(x)+R\psi(x)]\varphi(x'), & x>x'\end{cases}. \tag{2.7}$$

The function (2.7) satisfies automatically the first boundary condition in (2.4). The constants P and R are determined from the second boundary condition of (2.4) and from a relation that follows from Eq. (2.3) for the Green's function:

$$\frac{dG}{dx}(x+0,x)-\frac{dG}{dx}(x-0,x)=1.$$

As a result we get

$$G(xx')=-\varphi(x)\varphi(x')\left\{\frac{1/\varphi^2(d)}{\varkappa_d+\varphi'(d)/\varphi(d)}+\int_x^d\frac{dx_1}{\varphi^2(x_1)}\right\}, \quad x>x'; \qquad G(xx')=G(x'x), \quad x<x'. \tag{2.7a}$$

Here and below the prime denotes the derivative of φ with respect to x. The integral J_{tot} (2.2) the imaginary part of which is used to express the state density, is of the form

$$J_{tot}(p_\perp)=\int_0^d G(xx)\,dx = -\frac{1/\varphi^2(d)}{\varkappa_d+\varphi'(d)/\varphi(d)}\int_0^d\varphi^2(x)\,dx-\int_0^d\frac{dx}{\varphi^2(x)}\int_0^x\varphi^2(x_1)\,dx_1. \tag{2.8}$$

In the second of the integrals in the right-hand side we interchanged the order of the integration.

We shall make extensive use of the following lemma: all x satisfy the relation

$$\varphi'(x)\frac{d}{dE}\varphi(x)-\varphi(x)\frac{d}{dE}\varphi'(x)=\int_0^x\varphi^2(x_1)\,dx_1. \tag{2.9}$$

The proof is quite simple. We write down Eq. (2.5) for two energies E and $E+\Delta E$. Next, multiplying these relations respectively by $\varphi_{E+\Delta E}$ and φ_E and subtracting one from the other, we arrive as $\Delta E \to 0$ at Eq. (2.9).

Using relation (2.9), we easily represent (2.8) in the form

$$J_{tot}=\int_0^d G(xx)\,dx=\frac{d}{d\mu}\ln\left[\varphi(d)+\frac{1}{\varkappa_d}\varphi'(d)\right]. \qquad (2.10)$$

Substituting (2.10) in (2.2) and using the fact that $d\mu=-2p_\perp dp_\perp$, we obtain

$$g_\gamma(\mu)=-\frac{S}{(2\pi)^2}\,\mathrm{Im}\ln\left[\varphi(d)+\frac{1}{\varkappa_d}\varphi'(d)\right]_{p_\perp=0}. \qquad (2.10a)$$

In this relation it is necessary to choose for the total state density $g_\perp(\mu)$ only that branch of the logarithm which vanishes at $p_\perp=\infty$.

We consider now a more general situation, when we are interested in the state density of only a part ($0\leqslant x\leqslant d$) of the system, while the system occupies the region $0\leqslant x\leqslant d+t$. Let the potential on the segment $0\leqslant x\leqslant d$ have an arbitrary form $V(x)$, and let the potential at $d\leqslant x\leqslant d+t$ be constant and equal to V. In place of the second of the boundary conditions in (2.4), we assume the condition

$$\frac{dG}{dx}(d+t,x')+\sigma G(d+t,x')=0. \qquad (2.4a)$$

Then, using the lemma (2.9) and the explicit form of $\varphi(x)$ on the segment $d\leqslant x\leqslant d+t$:

$$\varphi(x)=\varphi'(d)\,\mathrm{sh}\,b(x-d)/b+\varphi(d)\,\mathrm{ch}\,b(x-d),$$

we obtain after simple identity transformations the following expression for the integral, in terms of whose imaginary part is the state density expressed on the segment $0\leqslant x\leqslant d$;

$$J_{loc}=\int_0^d G(xx)\,dx=\left\{\frac{d}{d\mu}\varphi(d)+\frac{1}{\varkappa_d}\frac{d}{d\mu}\varphi'(d)\right\}\Big/\left[\varphi(d)+\frac{1}{\varkappa_d}\varphi'(d)\right]. \qquad (2.11)$$

Here $\varkappa_d$ depends on μ and is of the form

$$\frac{1}{\varkappa_d}=\frac{1/\sigma+(1/b)\,\mathrm{th}\,bt}{1+(b/\sigma)\,\mathrm{th}\,bt},\qquad b=(V-E)^{1/2}. \qquad (2.12)$$

With the aid of (2.11), the state density of the region $0\leqslant x\leqslant d$ can be written in the form

$$g_\gamma(\mu)=-\frac{S}{2\pi^2}\int_0^\infty p_\perp\,dp_\perp$$

$$\times\mathrm{Im}\left\{\left[\frac{d}{d\mu}\varphi(d)+\frac{1}{\varkappa_d}\frac{d}{d\mu}\varphi'(d)\right]\Big/\left[\varphi(d)+\frac{1}{\varkappa_d}\varphi'(d)\right]\right\}. \qquad (2.11a)$$

Since $\varkappa_d$ depends now on $p_\perp$, we cannot take in (2.11a) the integral with respect to $p_\perp$ in general form, as was done in the derivation of (2.10a) for the total state density.

If the potential $V(x)$ is not constant on the segment $d\leqslant x\leqslant d+t$, then (2.12) is generalized in the following fashion:

$$1/\varkappa_d=-\tilde{\varphi}(d)/\tilde{\varphi}'(d). \qquad (2.13)$$

Here $\tilde{\varphi}(x)$ satisfies Eq. (2.5) with the following values on the boundary $(d+t)$:

$$\tilde{\varphi}(d+t)=-1/\sigma,\quad \tilde{\varphi}'(d+t)+\sigma\tilde{\varphi}(d+t)=0. \qquad (2.14)$$

Thus, Eq. (2.11a) enables us to calculate the state density of any part of the sandwich in terms of the characteristic function $\varphi(x)$. When the total state density of the entire system as a whole is calculated, substantial simplification is possible: integration is carried out with respect to the transverse momentum, and relation (2.10a) holds for the total state density. In the sections that follow we analyze with the aid of these relations the total and local state densities for the simplest systems.

III. TOTAL AND LOCAL STATE DENSITY IN AN ARBITRARY ONE-DIMENSIONAL POTENTIAL SATISFYING THE QUASICLASSICAL-ANALYSIS CONDITIONS

1. Total state density

We consider the total state density of the system $0\leqslant x\leqslant d$ with the general boundary conditions (2.4). The quasiclassical solution of Eq. (2.5) for the characteristic function with boundary conditions (2.6) at zero can be obtained, as usual[3]:

$$\varphi(x)=\frac{1}{[a(0)a(x)]^{1/2}}\,\mathrm{sh}\left[\int_0^x a(x_1)\,dx_1\right]+\frac{1}{\varkappa_0}\left[\frac{a(0)}{a(x)}\right]^{1/2}\mathrm{ch}\left[\int_0^x a(x_1)\,dx_1\right],$$

$$a(x)=[-(\mu-p_\perp^2-V(x)+i\gamma)]^{1/2},\quad \mathrm{Re}\,a|_{p_\perp^2=\infty}>0. \qquad (3.1)$$

Substituting (3.1) with $x=d$ in expression (2.10a) for the total state density, we obtain

$$g_\gamma(\mu)=g_V+g_S+g_{coh}, \qquad (3.2)$$

$$g_V=\frac{S}{4\pi^2}\Phi_r;\qquad \Phi_i-i\Phi_r=\int_0^d a(x)\,dx|_{p_\perp=0}, \qquad (3.2a)$$

$$g_S=\frac{S}{4\pi^2}\sum_{s=0,d}\left[\frac{\pi}{4}+\frac{1}{2}\,\mathrm{arctg}\frac{k_i(s)}{k_r(s)}-\mathrm{arctg}\frac{k_i(s)+\varkappa_s}{k_r(s)}\right], \qquad (3.2b)$$

$$k_i(s)-ik_r(s)=a(s)|_{p_\perp=0}\qquad (s=0,d),$$

$$g_{coh}=\frac{S}{4\pi^2}\,\mathrm{arctg}\frac{A\exp(-2\Phi_i)\sin 2(\Phi_r-\alpha)}{1-A\exp(-2\Phi_i)\cos 2(\Phi_r-\alpha)}, \qquad (3.2c)$$

$$A=\prod_{s=0,d}\left\{\frac{k_r^2(s)+(\varkappa_s-k_i(s))^2}{k_r^2(s)+(\varkappa_s+k_i(s))^2}\right\}^{1/2},$$

$$2\alpha=\sum_{s=0,d}\left[\mathrm{arctg}\frac{\varkappa_s-k_i(s)}{k_r(s)}+\mathrm{arctg}\frac{\varkappa_s+k_i(s)}{k_r(s)}\right]. \qquad (3.2d)$$

We note that to obtain $\varphi'(d)$ we need not differentiate the pre-exponential factor $a^{-1/2}(x)$ with respect to x, since $|a^{-2}da/dx|\ll 1$ is the principal quasiclassical approximation (see Ref. 3).

Equations (3.2)–(3.2d) describe the state density at arbitrary damping γ. The term g_V (3.2a) is the volume state density and is proportional to the average Fermi momentum of the system. The surface term g_S (3.2b) and the coherent g_{coh} (3.2c) is smaller by a factor $k_F d\gg 1$ than g_V. Then g_S is determined by the characteristics of the system only near the surface, and g_{coh} oscillates as a function of the total phase accumulated by the electron as it moves from one surface to the other. In the limiting case $2\Phi_i\gg 1$ the coherent term is exponentially small, $\sim\exp(-2\Phi_i)$, and we are left only with the terms g_V and g_S, in accord with the results of Balian and Bloch[1a] for the case of a constant potential. In the opposite limiting case $2\Phi_i\ll 1$, the quantity g_{coh} describes quantum oscillations of the state density (cf. Ref. 1b). When γ is varied, Eqs. (3.3) make it possible to trace the continuous transition from the pure quantum case to the completely smeared spectrum.

We emphasize that Eqs. (3.2) correspond to averaging of the state density over energy with width γ. The vanishing of the oscillating term g_{coh} upon averaging can be due to a number of different physical causes: scattering in the volume by impurities or other defects, or scattering by the boundaries of the system. The result actually does not depend on the averaging method, since the averaging affects only the coherent term and this term, as shown below, is built up uniformly only in the region where coherence is preserved. We consider the simplest averaging method, when the film is inhomogeneous over the thickness d and the results must be simply averaged over this thickness. We shall assume here that $V(x)$ does not depend on x. We let γ (meaning also k_i) tend to zero. Then averaging g_{coh} over the period of the oscillations yields zero:

$$\int_d^{d+\pi/k_r} dx\, g_{coh} = \int_d^{d+\pi/k_r} dx \operatorname{arctg}\frac{A\sin 2(k_r x-\alpha)}{1-A\cos 2(k_r x-\alpha)}$$

$$=\int_{-\infty}^{+\infty}\frac{dy}{1+y^2}\operatorname{arctg}\frac{2Ay}{(1-A)+(1+A)y^2}=0;\qquad y=\operatorname{tg}(k_r x-\alpha). \tag{3.3}$$

Thus, the result of averaging over the thickness corresponds exactly to the result of averaging over the energy with width γ, such that $\exp(-2\Phi_i)\ll 1$. In the case of a metal–semimetal sandwich (Sec. 4) we shall average over the thickness d of the metal and not over the energy, since averaging over the thickness simulates in simplest fashion the situation when there is no coherence when the electron moves in the metal, and the coherence is preserved when it moves in the semimetal.

2. Local state density

We examine now the accumulation of the various sections g_V, g_S, and g_{coh} of the total state density (3.2) at various points of space. Using formulas (2.11a) and (2.13), we can write for the state density g_{d_0} of the region $0\leqslant x\leqslant d_0$ the following expression:

$$g_{d_0}=-\frac{S}{2\pi^2}\operatorname{Im}\int_0^\infty p_\perp dp_\perp\left[\frac{d}{d\mu}\varphi(d_0)+\frac{1}{\varkappa_{d_0}}\frac{d}{d\mu}\varphi'(d_0)\right]\Big/\left[\varphi(d_0)+\frac{1}{\varkappa_{d_0}}\varphi'(d_0)\right],$$

$$1/\varkappa_{d_0}=-\tilde\varphi(d_0)/\tilde\varphi'(d_0); \tag{3.4}$$

$\varphi(d_0)$ and $\varphi'(d_0)$ are defined by relations (3.1). We can obtain similarly in the quasiclassical approximation the function $\tilde\varphi(x)$:

$$\tilde\varphi(x)=-\frac{1}{[a(d)a(x)]^{1/2}}\operatorname{sh}\int_x^d a(x_1)dx_1-\frac{1}{\varkappa_d}[a(d)/a(x)]^{1/2}\operatorname{ch}\int_x^d a(x_1)dx_1. \tag{3.5}$$

We substitute (3.1) and (3.5) in (3.4) and separate in the latter those terms that contain in the numerator the following hyperbolic functions:

$$\operatorname{sh}\int_x^d a(x_1)dx_1,\quad \operatorname{ch}\int_x^d a(x_1)dx_1,$$

$$\operatorname{sh}\int_0^x a(x_1)dx_1,\quad \operatorname{ch}\int_0^x a(x_1)dx_1.$$

This expression will be designated $\Delta g_S(d_0)$. We subdivide the remaining expression, which contains both in the numerator and in the denominator only the hyperbolic functions

$$\operatorname{sh}\int_0^d a(x_1)dx_1,\quad \operatorname{ch}\int_0^d a(x_1)dx_1,$$

into two parts in the following manner. The first part is obtained by replacing these hyperbolic functions in the expression by unity, and the second is the remainder. Recognizing that $d\mu=-2ada$, the first part is evaluated in explicit form and contributes to the volume and surface parts g_V and g_S of the state density. The second part contributes to the coherent term g_{coh} and is calculated by changing over to the complex plane of the variable $p_\perp^2=x-iy$ $(y>0)$ along the contour shown in Fig. 2. It is easily seen that the integral along the arc in the complex plane vanishes when the arc tends to infinity, and the integral along the imaginary axis builds up in a narrow region of the variable y (at $x=0$). Expanding a near $y=0$ and taking into account the dependence of a on y only under the exponential sign (with accuracy $\sim 1/\mu^{1/2}d$), we can evaluate the integral exactly in the limit $\mu^{1/2}d\gg 1$. Results for g_{d_0} takes the form

$$g_{d_0}=g_V(d_0)+g_S(d_0)+g_{coh}(d_0), \tag{3.6}$$

$$g_V(d_0)=\frac{S}{4\pi^2}\Phi(d_0),\qquad \Phi(d_0)=-\operatorname{Im}\int_0^{d_0}a(x)dx|_{p_\perp=0}, \tag{3.6a}$$

$$g_S(d_0)=\frac{S}{4\pi^2}\left[\frac{\pi}{4}+\frac{1}{2}\operatorname{arctg}\frac{k_i(0)}{k_r(0)}-\operatorname{arctg}\frac{\varkappa_0+k_i(0)}{k_r(0)}\right]+\Delta g_S(d_0), \tag{3.6b}$$

$$g_{coh}(d_0)=\frac{S}{4\pi^2}\operatorname{Re}\left(\frac{T_0}{T}\right)\operatorname{arctg}\frac{A\exp(-2\Phi_i)\sin 2(\Phi_r-\alpha)}{1-A\exp(-2\Phi_i)\cos 2(\Phi_r-\alpha)}+\Delta g_{coh}(d_0);$$

$$\frac{T_0}{T}=\int_0^{d_0}\frac{dx}{a(x)}\Big/\int_0^d\frac{dx}{a(x)}\Big|_{p_\perp=0}, \tag{3.6c}$$

where T_0/T is the ratio of the time of stay of the electron in the region d_0 to the period of motion from one boundary of the sandwich to the other;

$$\Delta g_{coh}(d_0)=-\frac{S}{4\pi^2}\operatorname{Im}\left(\frac{T_0}{T}\right)\ln|1+A^2\exp(-4\Phi_i)$$

$$-2A\exp(-2\Phi_i)\cos 2(\Phi_r-\alpha)|. \tag{3.6d}$$

The term $\Delta g_{coh}(d_0)$ (3.6d), is generally speaking small. It vanishes identically in a constant potential, and also at $\gamma=0$. In addition, $\Delta g_{coh}(d)\equiv 0$.

The term $\Delta g_S(d_0)$ can be analyzed in perfect analogy with $g_{coh}(d_0)$ along the contour of Fig. 2. It is easily seen that it is significant only at distances on the order of the wavelength near the system boundaries. In the remaining region it is small and is of the order of $\sim S/\mu^{1/2}d_0$. The behavior of $\Delta g_S(d_0)$ at small thicknesses makes it possible to trace precisely the buildup of $g_S(d_0)$ over distances of the order of a wavelength near the surface.

Thus, the volume term $g_V(d_0)$ (3.6a) is built up uniformly over the volume in proportion to the momentum

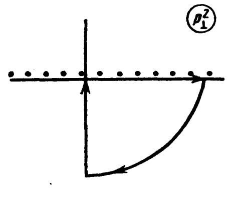

FIG. 2.

$k_r(x)$ in the corresponding part of space. The surface term $g_S(d_0)$ (3.6b) is completely built up over distances d_0 of the order of the wavelength ($\sim 1/\mu^{1/2}$), since, as noted above, $\Delta g_S(d_0)$ falls off over distances larger than the wavelength like $1/\mu^{1/2}d_0$. The coherent term $g_{coh}(d_0)$ (3.6c) accumulates in proportion to the time of stay in the corresponding layer and is inversely proportional to the momentum. The period of the oscillations of $g_{coh}(d_0)$ is determined by the total phase accumulated on the entire trajectory of the motion.

IV. STATE DENSITY IN METAL-SEMIMETAL SYSTEMS

In the preceding section we considered the state density of the system when the potential varies sufficiently slowly along the system: over distances on the order of the wavelength, the Fermi momentum changes by an amount much less than unity. In real junctions between two different metals, the situation is usually the inverse: the Fermi momentum changes by a value of the order of unity over distances of the order of the wavelength, and at the metal–semimetal junction the momentum changes by a large factor. As the starting model of such a junction we consider therefore the case when the potential changes jumpwise (cf. Fig. 1):

$$V(x)=\begin{cases}0, & 0\leqslant x\leqslant d.\\ V, & d\leqslant x\leqslant d+t.\end{cases}\tag{4.1}$$

We are interested in the situation described in the introduction and formulated in a paper by Kagan and the author,[2] when the electron moves coherently in a semimetal of thickness t, while coherence is violated in the metal of thickness d. We shall simulate this by averaging the final result over the thickness of the metal d. The averaging over the energy with width γ, carried out in Sec. 3, leads, generally speaking, to violation of coherence both in the metal and in the semimetal. However, if the thickness of the semimetal t is small enough compared with the thickness d of the metal (more accurately, if $t/p \ll d/k$; k is the Fermi momentum in the metal and p is the Fermi momentum in the semimetal), then we can choose an energy width $\gamma(\gamma d/k \gg 1$, but with $\gamma t/p \ll 1)$, the smearing of the state density over which does not violate the coherence of the motion in the semimetal, and there is no coherence over the thickness of the metal at all. In this case the averaging over the thickness of the metal is fully equivalent to averaging over energy with such a width γ.

1. Total state denstiy of metal-semimetal system

For the potential (4.1) we can easily write down the characteristic function $\varphi(x)$ in explicit form:

$$\varphi(x)=\begin{cases}\dfrac{\operatorname{sh} ax}{a}+\dfrac{\operatorname{ch} ax}{\varkappa_0}, & 0\leqslant x\leqslant d\\[2ex] \varphi'(d)\dfrac{\operatorname{sh} b(x-d)}{b}+\varphi(d)\operatorname{ch} b(x-d), & d\leqslant x\leqslant d+t\end{cases},\tag{4.2}$$

$$a=[-(\mu-p_\perp^2+i\gamma)]^{1/2},$$
$$b=[-(\mu-V-p_\perp^2+i\gamma)]^{1/2}.$$

For the total state density of the entire system we have the relation

$$g_{tot}=-\frac{S}{4\pi^2}\operatorname{Im}\ln\left[\varphi(d+t)+\frac{1}{\sigma}\varphi'(d+t)\right].\tag{4.3}$$

Here σ is the boundary condition [see (2.4a)] on the boundary $(d+t)$. Substituting from (4.2) the values of the characteristic function at the point $(d+t)$, we can represent g_{tot} in a form similar to (3.2). We shall carry out the averaging of the obtained expression over the thickness of the metal d. The averaging reduces to a calculation of exactly the same integrals as in (3.3). It is easy to note that the result of the averaging corresponds to replacing in (4.3) the hyperbolic functions $\sinh ad$ and $\cosh ad$ by $\frac{1}{2}e^{ad}$ [the same was done also in the averaging of expression (3.2)]. As a result we obtain for the total state density averaged over the metal thickness d (as $\gamma \to 0$)

$$\langle g_{tot}\rangle=g_V+g_S+\langle g_{coh}\rangle,\tag{4.4}$$

$$g_V=(S/4\pi^2)(kd+pt),\tag{4.4a}$$

$$g_S=\frac{S}{4\pi^2}\left(\frac{\pi}{2}-\operatorname{arctg}\frac{\varkappa_0}{k}-\operatorname{arctg}\frac{\sigma}{p}\right),\tag{4.4b}$$

$$\langle g_{coh}\rangle=-\frac{S}{4\pi^2}\operatorname{arctg}\frac{C\sin 2(pt-\alpha)}{1+C\cos 2(pt-\alpha)},\tag{4.4c}$$

$$C=\frac{k-p}{k+p},\qquad \alpha=\operatorname{arctg}\frac{\sigma}{p}.$$

Here g_V is the volume state density in the potential (4.1), cf. (3.2a); g_S is the surface state density in the potential (4.1), cf. (3.2b); $\langle g_{coh}\rangle$ is the coherent part of the state density averaged over the metal thickness. We see that $\langle g_{coh}\rangle$ oscillates as a function of the semimetal thickness t (the ordinates in Fig. 3 are given in units of $S/4\pi^2$). At $p \ll k$ the amplitude of the oscillations is close to $\pi/2$, since $C\approx 1$. At $p=k$ the oscillations naturally disappear, inasmuch as in a constant potential it does not matter whether we average the state density over the region d or over the region $(d+t)$.

We consider now the accumulation of the oscillating part of the state density $\langle g_{coh}\rangle$ in various parts of the system.

2. State density of metallic layer in a metal-semimetal system

For the state density of the metal in a metal–semimetal system we can use Eq. (2.11a):

$$g_{met}=-\frac{S}{2\pi^2}\int_0^\infty p_\perp\,dp_\perp\operatorname{Im}\left\{\left[\frac{d}{d\mu}\varphi(d)+\frac{1}{\varkappa_d}\frac{d}{d\mu}\varphi'(d)\right]\Big/\left[\varphi(d)+\frac{1}{\varkappa_d}\varphi'(d)\right]\right\},\tag{4.5}$$

$$\frac{1}{\varkappa_d}=\frac{1/\sigma+(1/b)\operatorname{th} bt}{1+(b/\sigma)\operatorname{th} bt}.\tag{4.5a}$$

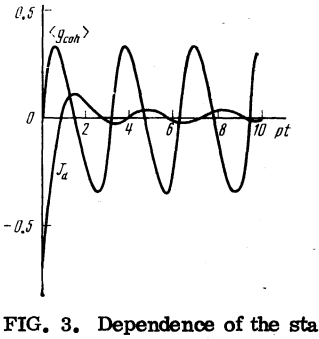

FIG. 3. Dependence of the state density on the thickness of the semimetal ($\sigma=\infty$, $(\mu-V)/\mu=0.25$).

The analysis of relations (4.5) and (4.5a) is perfectly analogous to the analysis of expression (3.4). It is useful to separate from (4.5) the part obtained by replacing the hyperbolic functions $\sinh ad$ and $\cosh ad$ by unity. The remaining expression can be easily shown to vanish after averaging over the thickness d of the metal. This is easiest to see in the case when the metal thickness d is large enough compared with the semimetal thickness t, or more accurately

$$d/k \gg t/p. \tag{4.6}$$

In this case the dependence of $\varkappa_d$ in (4.5a) on the momentum $p_\perp^2$ can be neglected, and the integral can be evaluated in exactly the same manner as the integral that leads to the term $g_{coh}(d_0)$ in (3.6c). In this case $\varkappa_d$ appears at $p_\perp^2=0$. The averaging of the resultant expression over d was carried out in (3.3) and yielded zero. Actually it can be shown that the restriction (4.6) is immaterial, and at all $kd \gg 1$ the resultant expression vanishes upon averaging. This is seen, in particular, directly in the limiting case that is the inverse of (4.6), when $d/k \ll t/p$. In this case the quantity $\tanh bt$ in $\varkappa_d$ (4.5a) can be set identically equal to unity, and the integral can be again evaluated, just as in the case $g_{coh}(d_0)$ (3.6c). Thus, we see that to average the integrals over the thickness d of the metal it is sufficient to replace the quantities $\sinh ad$ and $\cosh ad$ in the integrand by the quantity $\frac{1}{2}e^{ad}$. As a result we obtain for the averaged state density of the metallic layer

$$\langle g_{met}\rangle = g_{V\,met}+g_{S\,met}, \tag{4.7}$$

$$g_{V\,met}=Skd/4\pi^2, \tag{4.7a}$$

$$g_{S\,met}=\sum_{s=0,d} J_s, \tag{4.7b}$$

$$J_s=\frac{S}{8\pi^2}\operatorname{Im}\int_0^\infty \frac{dp_\perp^2}{a^2}\left\{\frac{1}{2}-\frac{1}{1+a/\varkappa_s}\right\}, \qquad s=0,\ d. \tag{4.8a}$$

The quantity J_0 is the surface contribution of the free metallic surface [cf. (4.4b)]:

$$J_0=\frac{S}{4\pi^2}\left(\frac{\pi}{4}-\operatorname{arctg}\frac{\varkappa_0}{k}\right), \tag{4.8b}$$

J_d is the surface contribution from the metallic surface in contact with the semimetal. We change J_d to a somewhat more convenient form. We note for this purpose that the integral

$$J(V)=\frac{S}{8\pi^2}\operatorname{Im}\int_0^\infty \frac{dp_\perp^2}{a^2}\,\frac{1}{1+a/b} \tag{4.9}$$

does not depend on V and is equal to the first of the integrals in the curly brackets of (4.8a). That this is actually the case can be verified directly, since the integral in (4.9) is evaluated in explicit form, for example, with the aid of the Euler substitution

$$u=a+(a^2+V)^{1/2} \quad (dp_\perp^2=2a\,da).$$

Thus, J_d can be rewritten in the form

$$J_d=-\frac{S}{8\pi^2}\operatorname{Im}\int_0^\infty \frac{dp_\perp^2}{a^2}\left[1\Big/\left(1+\frac{a}{\varkappa_d}\right)-1\Big/\left(1+\frac{a}{b}\right)\right]. \tag{4.10}$$

The expression in this form is convenient because it shows that as $t\to\infty$, regardless of the value of σ, the integral J_d tends to zero. The integral of J_d cannot be evaluated directly, but it can be easily calculated numerically. At small $t\,(pt\lesssim 1)$ the form (4.10) of J_d is quite convenient for numerical calculation. At larger t $(pt\gtrsim 1)$ it is more useful to transform the integral of (4.10) along the contour of Fig. 2. As a result we get

$$J_d=\frac{S}{4\pi^2}\operatorname{Re}\int_0^\infty dy\,\frac{b}{a}\left\{e^{2bt}\frac{1+b/\sigma}{1-b/\sigma}(a+b)^2\mp V\right\}^{-1},$$

$$b=[-(\mu-V+iy)]^{1/2},\quad a=[-(\mu+iy)]^{1/2},\quad p=(\mu-V)^{1/2}. \tag{4.10a}$$

At $t\gtrsim 1/p$ expression (4.10a) is perfectly convenient for a numerical calculation, since the integral is concentrated mainly in the region $y\sim p/t$. The results of numerical calculation are shown in Fig. 3. In the limit $pt\gg 1$ the integral (4.10a) can be evaluated exactly:

$$J_d|_{pt\gg1}=\frac{S}{8\pi^2}\,\frac{\mu-V}{\mu^{1/2}tV}\ln\left|1+B^2-2B\cos 2\left(pt+\operatorname{arctg}\frac{p}{\sigma}\right)\right|, \tag{4.10b}$$

$$B=V/(k+p)^2,\quad k=\mu^{1/2}.$$

Our analysis shows that J_d does not have a small quantity in the parameter $kd\gg 1$ compared with $\langle g_{coh}\rangle$ (4.4c). However, for sufficiently large $t\,(pt\gtrsim 1)$ the integral in J_d has a specific smallness for two reasons. First, J_d contains the ratio $(\mu-V)/\mu$. Second, there is built up in J_d a numerical smallness compared with $\langle g_{coh}\rangle$ because $\langle g_{coh}\rangle$ contains the arctangent of (4.4c), the characteristic changes of which are of the order of π, while J_d contains at large t the natural logarithm of (4.10b), with a characteristic variation ~1.

We see thus that the averaged state density of the metal (4.7) consists of a volume term and of the surface terms (4.8). The surface term J_d from the region adjacent to the semimetal has an oscillatory dependence on the thickness of the semimetal. The amplitude of these oscillations is numerically somewhat smaller than the amplitude of the oscillations of the total state density $\langle g_{coh}\rangle$ (4.4c). In perfect analogy with Sec. III.2, we can trace the locations where individual terms of the state density of the metal (4.7) are built up. The volume term $g_{V\,met}$ is built up uniformly over the entire metal. The surface terms J_0 and J_d are built up at a distance on the order of wavelength $(1/k)$ near the corresponding metal boundary. Thus, the semimetal forms in the region of the contact with the metal a new boundary condition, which depends in oscillatory manner on the thickness t of the semimetal layer, and information on the presence of the semimetal layer penetrates to a distance of the order of the wavelength into the metal.

3. State density of semimetallic layer

To obtain the state density of the semimetallic layer it is necessary to use formula (2.11a) twice, for the entire system as a whole and separately for the metallic layer, respectively, and to subtract one expression from the other. After straightforward transformations we obtain the density g_t of the states of the semimetallic layer. Averaging g_t over the thickness of the metal is carried out just as in Sec. IV.2. It is then easy to see that the state density of the semimetallic layer, averaged over the thickness of the metal, reduces to the form

$$\langle g_t\rangle=\frac{S}{4\pi^2}\left\{pt+\frac{\pi}{4}-\operatorname{arctg}\frac{\sigma}{p}+\operatorname{arctg}\frac{C\sin 2(pt-\alpha)}{1+C\cos 2(pt-\alpha)}\right\}-J_d; \tag{4.11}$$

$\langle g_t \rangle$ and $\langle g_{met} \rangle$ (4.7) yield together in natural fashion the total averaged state density $\langle g_{tot} \rangle$ (4.4).

4. Quasiclassical analysis

Let the potential $V(x)$ vary in the region of the semimetal ($d<x<d+t$) slowly, so as to satisfy the quasiclassical conditions

$$\frac{d}{dx}\frac{1}{b(x)} \ll 1, \quad b(x)=[-(\mu-V(x)+i\gamma)]^{1/2}. \tag{4.12}$$

In this case the characteristic function $\varphi(x)$ is written in analogy with (4.2), and at the point $x=d$ it is joined with the function of the form (3.1) with replacement of $a(x)$ by $b(x)$. We write down the total density of states of this system, averaged over the thickness of the metal. In analogy with (4.4) we have

$$\langle g_{tot} \rangle = g_V + g_S + \langle g_{coh} \rangle, \tag{4.13}$$

$$g_V = S(kd+\chi)/4\pi^2, \tag{4.13a}$$

$$g_S = \frac{S}{4\pi^2}\left(\frac{\pi}{2} - \operatorname{arctg}\frac{\varkappa_0}{k} - \operatorname{arctg}\frac{\sigma}{p(d+t)}\right), \tag{4.13b}$$

$$\langle g_{coh} \rangle = -\frac{S}{4\pi^2}\operatorname{arctg}\frac{C\sin 2(\chi-\alpha)}{1+C\cos 2(\chi-\alpha)}. \tag{4.13c}$$

Here

$$\chi = i\int_d^{d+t} b(x)\,dx|_{p_\perp=0,\gamma=0}, \qquad p(x)=ib(x)|_{p_\perp=0,\gamma=0} \qquad (x=d,\, d+t),$$

$$C=\frac{k-p(d)}{k+p(d)}, \qquad \alpha=\operatorname{arctg}\frac{\sigma}{p(d+t)} .$$

The period χ of the oscillations is determined by the total phase accumulated by the electrons in the semimetal along a trajectory with zero transverse momentum $p_\perp=0$ and with an energy equal to the Fermi energy. In analogy with the treatment in the preceding two sections, IV.1 and IV.2, we can show that the oscillating part of the state density builds up uniformly in the region of the semimetal in proportion to the time of stay of the electron on the corresponding section of the quasiclassical trajectory ($\sim 1/p(x)$, cf. the analysis in Sec. III.2), while in the metal in the region of the contact with the semimetal the oscillating part attenuates over distances of the order of the electron wavelength in the metal.

We note the important fact that when averaged over the thickness of the metal the oscillations do not vanish only if the potential varies sufficiently rapidly in the region of the contact between the metal and semimetal. It is seen from (4.13c) that if the jump of the potential at the metal–semimetal interface is equal to zero ($p=k$), then $C=0$ and the oscillations vanish. More accurately, if $p=k$ we can show that the oscillations appear only in the approximation that follows the approximation in the quasiclassical parameter (4.12), and furthermore only in the case when the derivative of the potential has a discontinuity. In other words, it can be stated that if the potential $V(x)$ varies slowly in the region of the contact between the metal and the semimetal over distances of the order of the wavelength of the electron, then the averaging of the state density over the metal thickness leads to a complete vanishing of the oscillations. In the opposite limiting case, when the Fermi momentum in the region of the junction changes substantially over distances much smaller than the wavelength, it is easily seen that the oscillations do not vanish upon averaging—this case reduces in fact to the potential (4.1) and can be treated by perturbation theory. For example, in the case $\sigma=\infty$ we can obtain

$$C=[k-p-\rho(k+p)]/[k+p-\rho(k-p)].$$

Here ρ is a small parameter that characterizes the narrow transition region between the metal and the semimetal. If the potential varies linearly in the region of the contact at $d-l<x<d+l$, then this parameter takes the form $\rho=Vl^2/6$.

Thus, oscillations of the averaged state density take place only when the potential in the region of the contact varies rapidly enough: at distances on the order of the wavelength the Fermi momentum should change by at least a value on the order of unity. As already noted by us, it is precisely this situation that takes place usually in metallic contacts.

The first to observe oscillations of the different measured quantities as functions of the thickness t of the semimetal were Mikheeva *et al.* (for details see Refs. 2 and 4).

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