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LETTER TO THE EDITOR

Semiclassical theory in Andreev billiards: beyond the diagonal approximation

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Abstract
Recently semiclassical approximations have been successfully applied to study the effect of a superconducting lead on the density of states and conductance in ballistic billiards. However, the summation over classical trajectories involved in such theories was carried out using the intuitive picture of Andreev reflection rather than semiclassical reasoning. We propose a method to calculate the semiclassical sums which allows us to go beyond the diagonal approximation in these problems. In particular, we address the question of whether the off-diagonal corrections could explain the gap in the density of states of a chaotic Andreev billiard.

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1. Introduction

Andreev billiards are two-dimensional electron cavities with a superconducting part of the boundary (see [1] for a review). A negatively charged electron incident on the superconductor is reflected as a positively charged hole with an opposite momentum. This process of Andreev reflection [2] generates a new kind of dynamics in comparison to conventional (normal) billiards. The excitation spectrum of an Andreev billiard depends on the shape of its boundary [3, 4]. Using the random-matrix theory, it was shown [3] that the density of states (DoS) $d(E)$ in the chaotic billiard has a minigap around the Fermi energy E_F, while in the integrable billiard it is proportional to E, the energy counted from E_F. The width of the minigap is of the order of the Thouless energy, which is much smaller than the superconducting gap Δ. The semiclassical theory of [4] confirms the above results in the integrable case, but finds an exponential suppression of $d(E)$, instead of a gap, in the chaotic cavity. The authors surmised that the disagreement can be attributed to the use of diagonal approximation. The method proposed below allows one to determine the off-diagonal corrections in a billiard with a superconducting lead. (A somewhat similar concept was used in [5] in the case where the

whole boundary is superconducting.) We find that these corrections may, indeed, reflect the existence of the gap, although the full understanding of the problem is still missing.

Another area of the application of the semiclassical techniques is transport problems. In general, the conductance of a billiard with a superconducting lead can be expressed in terms of transmission and reflection amplitudes with or without electron-to-hole conversion [6, 7]. In particular, the contribution of the Andreev reflection to the conductance is proportional to $R_A \equiv \mathrm{Tr}\big(r_{he} r_{he}^{\dagger}\big)$, where r_{he} is a part of the scattering matrix describing an electron injected into the billiard returning back as a hole. In [8], this quantity was calculated semiclassically under the assumption of the exact Andreev reflection ($E \to 0$) for a three-probe geometry. Both the diagonal and off-diagonal (weak localization) contributions were given. It was argued there that R_A is equal simply to the normal transmission coefficient for an electron to reach the superconducting lead (then, classically, it would return back as a hole with a 100% probability). Hence, the off-diagonal corrections to R_A could be computed by standard methods [9] developed for a normal billiard. In this letter, we start from the *quantum* relation [10] between R_A and the normal transmission amplitudes (in the case of a two-probe geometry) and then apply the semiclassical limit. Thus, no additional classical assumption is required. It is found that, while the diagonal part of R_A is, in fact, equal to the classical normal transmission, the weak-localization correction is nontrivial.

2. Density of states

2.1. Problems with the earlier approach

Here, we outline the semiclassical theory of [4] and point out the technical difficulties that arise when sums over classical trajectories are calculated. We consider a chaotic billiard with a superconducting lead. The lead width w is assumed to be small compared to the perimeter of the billiard, so as not to spoil its chaoticity. The energy is taken to be high enough to provide for a large number of open channels $N = k_F w/\pi \gg 1$ in the lead (k_F is the Fermi wave number). The lead is modelled as an ideal wire connecting the billiard and the superconductor. The average quasiparticle DoS is given by [4]

$$d(E) = d_0 - \frac{1}{\pi}\,\mathrm{Im}\sum_{l=1}^{\infty}\frac{(-1)^l}{l}\frac{\partial}{\partial E}\langle \mathrm{Tr}[S(E)S^*(-E)]^l\rangle, \tag{1}$$

where $d_0 = M\mathsf{A}/2\pi\hbar^2$ is the average DoS for a particle of mass M in the isolated billiard of area A, $S(E)$ is the electron scattering matrix for the billiard with the normal lead, the energy E is measured from E_F and the average is taken over a classically small interval of k_F. In the semiclassical approximation, the scattering matrix [11, 12]

$$S_{nm}(E) = \sum_{\gamma(n,m)} \mathcal{A}_\gamma \exp\left(\frac{\mathrm{i}}{\hbar}\mathcal{S}_\gamma\right) \tag{2}$$

is a sum over classical trajectories $\gamma(n, m)$ starting and ending at the lead and connecting the channels m and n. The trajectories make an angle $\theta_m = \pm\sin^{-1}(m\pi/k_F w)$ with the lead direction as they enter the billiard, and θ_n—as they leave it. Here we assumed $|E| \ll E_F$. The actions then can be expanded about E_F as $\mathcal{S}_\gamma(E) \simeq \mathcal{S}_\gamma(0) + E\mathcal{T}_\gamma(0)$, where $\mathcal{T}_\gamma$ is the time and

$$\mathcal{S}_\gamma(p_n, p_m; E = 0) = \int_\gamma \mathbf{p}\cdot \mathrm{d}\mathbf{r} - p_n y_n + p_m y_m \tag{3}$$

is in the momentum representation on the lead. Here, $y_{m(n)}$ are initial (final) coordinates at the lead cross section and $p_{m(n)} = \hbar k_F \sin\theta_{m(n)}$ are the conjugate momenta. The prefactors $\mathcal{A}_\gamma = |\mathcal{A}_\gamma| \exp(-\mathrm{i}\mu_\gamma \pi/2)$ depend on the Maslov indices μ_γ and

$$|\mathcal{A}_\gamma| = \left(\frac{\pi}{2k_F w^2}\left|\frac{\partial y_n}{\partial(\sin\theta_m)}\right|\right)^{1/2} = \left(\frac{\pi\hbar}{2w^2}\left|\frac{\partial^2 S_\gamma}{\partial p_n \partial p_m}\right|\right)^{1/2}. \tag{4}$$

Using the semiclassical expression (2), the authors of [4] arrive, in the diagonal approximation, at the following result:

$$\begin{aligned}\langle \mathrm{Tr}[S(E)S^*(-E)]^l\rangle &= \sum_{n,m=1}^{N}\sum_{\gamma(n,m)} |\mathcal{A}_\gamma|^2 \exp\left(\frac{\mathrm{i}}{\hbar}2lE\mathcal{T}_\gamma\right)\\ &\simeq \frac{k_F}{2\pi}\int_{-1}^{1}\mathrm{d}(\sin\theta)\int_0^w \mathrm{d}y \exp\left[\frac{\mathrm{i}}{\hbar}2lE\mathcal{T}(y,\theta)\right],\end{aligned} \tag{5}$$

where the sums become the integrals over the initial (or final) conditions (y,θ) in the limit $N \gg 1$. While the derivation of this formula for $l = 1$ is given in [4], its generalization to $l > 1$ is not obvious. For example, when $l = 2$, we can write

$$\begin{aligned}\mathrm{Tr}[S(E)S^*(-E)]^2 = &\sum_{\substack{n_1,n_1',\\ n_2,n_2'=1}}^{N}\sum_{\substack{\gamma_1(n_1,n_1'),\gamma_1'(n_1',n_2),\\ \gamma_2(n_2,n_2'),\gamma_2'(n_2',n_1)}} \mathcal{A}_{\gamma_1}\mathcal{A}^*_{\gamma_1'}\mathcal{A}_{\gamma_2}\mathcal{A}^*_{\gamma_2'}\\ &\times \exp\left[\frac{\mathrm{i}}{\hbar}\left(\mathcal{S}_{\gamma_1} - \mathcal{S}_{\gamma_1'} + \mathcal{S}_{\gamma_2} - \mathcal{S}_{\gamma_2'}\right)\right]\exp\left[\frac{\mathrm{i}}{\hbar}E\left(\mathcal{T}_{\gamma_1} + \mathcal{T}_{\gamma_1'} + \mathcal{T}_{\gamma_2} + \mathcal{T}_{\gamma_2'}\right)\right].\end{aligned} \tag{6}$$

After this expression is averaged over a small window of k_F, only the terms where the actions cancel in the exponent will remain. The diagonal approximation amounts to keeping the terms with all four actions equal. In a chaotic system without symmetries this is only possible when $\gamma_1 = (\gamma_1')^{-1} = \gamma_2 = (\gamma_2')^{-1}$, where γ^{-1} is the time-reversed path γ. This condition corresponds to the exact Andreev reflection at $E = 0$. It yields the average

$$\langle \mathrm{Tr}[S(E)S^*(-E)]^2\rangle = \sum_{n,n'}\sum_{\gamma(n,n')} |\mathcal{A}_\gamma|^4 \exp\left(\frac{\mathrm{i}}{\hbar}4E\mathcal{T}_\gamma\right), \tag{7}$$

which is a wrong result. Thus, this calculation shows that the diagonality requirement alone is not sufficient in the case of Andreev billiards. As we shall see next, the stationary-phase (SP) approximation must be employed when calculating the semiclassical sums.

2.2. *Traces of scattering matrices*

In this section, we derive equation (5) and find the quantum corrections to it. In order to focus on the idea of the method, the case $l = 2$ is considered here and the general situation is treated in appendix A.1.

2.2.1. Classical contribution. We begin by rewriting the channel sum (6) as an integral over momenta

$$\begin{aligned}\mathrm{Tr}[S(E)S^*(-E)]^2 = &\left(\frac{w}{\pi\hbar}\right)^4 \int_{-\hbar k_F}^{\hbar k_F} \mathrm{d}p_1\,\mathrm{d}p_1'\,\mathrm{d}p_2\,\mathrm{d}p_2' \sum_{\substack{\gamma_1,\gamma_1',\\ \gamma_2,\gamma_2'}} \mathcal{A}_{\gamma_1}\mathcal{A}^*_{\gamma_1'}\mathcal{A}_{\gamma_2}\mathcal{A}^*_{\gamma_2'}\\ &\times \exp\left[\frac{\mathrm{i}}{\hbar}\left(\mathcal{S}_{\gamma_1} - \mathcal{S}_{\gamma_1'} + \mathcal{S}_{\gamma_2} - \mathcal{S}_{\gamma_2'}\right)\right]\exp\left[\frac{\mathrm{i}}{\hbar}E\left(\mathcal{T}_{\gamma_1} + \mathcal{T}_{\gamma_1'} + \mathcal{T}_{\gamma_2} + \mathcal{T}_{\gamma_2'}\right)\right].\end{aligned} \tag{8}$$

Although each channel allows for two signs of the momentum, it is expected that the leading contribution to the integral comes from the Andreev-reflected paths. Therefore, given p_1, p_1', p_2 and p_2', the initial and final momenta of the four paths are set as follows: $\gamma_1(p_1 \leftarrow -p_1')$, $\gamma_1'(p_1' \leftarrow -p_2)$, $\gamma_2(p_2 \leftarrow -p_2')$ and $\gamma_2'(p_2' \leftarrow -p_1)$.

It is convenient to compute the integral (8) in the rotated coordinates:

$$\begin{cases} a = \dfrac{p_1 - p_2}{\sqrt{2}} \\ b = \dfrac{p_1 + p_2}{\sqrt{2}} \end{cases} \quad \text{and} \quad \begin{cases} a' = \dfrac{p_1' - p_2'}{\sqrt{2}} \\ b' = \dfrac{p_1' + p_2'}{\sqrt{2}}. \end{cases} \tag{9}$$

It will be possible to integrate over $\mathrm{d}a\,\mathrm{d}a'$ in the SP approximation. Consider the phase function

$$\Phi(a, b, a', b') \equiv \mathcal{S}_{\gamma_1}(p_1, -p_1') - \mathcal{S}_{\gamma_1'}(p_1', -p_2) + \mathcal{S}_{\gamma_2}(p_2, -p_2') - \mathcal{S}_{\gamma_2'}(p_2', -p_1), \tag{10}$$

where the momenta must be expressed in terms of the new coordinates. It is easy to show that the SP condition $\partial\Phi/\partial a = \partial\Phi/\partial a' = 0$ can be rewritten as a relation between the initial and final positions $y^{i,f}$ of the trajectories on the lead:

$$-y^f_{\gamma_1} - y^i_{\gamma_1'} + y^f_{\gamma_2} + y^i_{\gamma_2'} = -y^i_{\gamma_1} + y^f_{\gamma_1'} + y^i_{\gamma_2} - y^f_{\gamma_2'} = 0. \tag{11}$$

These equations are satisfied if

$$\gamma_1 = \gamma_2 \qquad \text{and} \qquad \gamma_1' = \gamma_2', \tag{12}$$

and the stationary point is given by $a = a' = 0$. Now it is necessary to employ the diagonal-approximation requirement $\Phi = 0$. It limits possible trajectories to $\gamma_1 = (\gamma_1')^{-1} = \gamma_2 = (\gamma_2')^{-1}$, as expected. Since the condition $\Phi = 0$ is fulfilled for arbitrary b and b', the integral over $\mathrm{d}b\,\mathrm{d}b'$ must be performed exactly. In the original coordinates, it is the integral over the manifold:

$$\begin{cases} p_1 = p_2 \\ p_1' = p_2' \end{cases} \quad (|p_i|, |p_i'| \leqslant k_F). \tag{13}$$

To complete the program, we compute the second derivatives of the phase at the SP point:

$$\left.\frac{\partial^2\Phi}{\partial a^2}\right|_{a=a'=0} = \left.\frac{\partial^2\Phi}{\partial a'^2}\right|_{a=a'=0} = 0, \qquad \left.\frac{\partial^2\Phi}{\partial a\partial a'}\right|_{a=a'=0} = 2\frac{\partial^2\mathcal{S}_{\gamma_1}(p_1, -p_1')}{\partial p_1 \partial(-p_1')}. \tag{14}$$

The SP integration leads to the cancellation of $|\mathcal{A}_{\gamma_1}|^2$ in (8), according to (4). Finally, transforming the $\mathrm{d}b\,\mathrm{d}b'$ integral to the $\mathrm{d}p_1\,\mathrm{d}p_1'$ integral, we arrive at (5).

It is instructive to consider an analogy with the semiclassical treatment of normal reflection. Suppose, the scattering matrix S_1 (S_2) describes the propagation of the particle before (after) the reflection and $S = S_2 S_1$ is the total scattering matrix. Semiclassically, S_1 and S_2 are given as sums over classical trajectories. If S is calculated in the SP approximation, it will be a sum over combined classical trajectories which include the reflection. In the case of Andreev billiard, the consequence of the SP approximation is the equality of trajectories (12), while the Andreev reflection is required by the diagonal approximation.

2.2.2. Quantum corrections. There are two types of quantum corrections to (5): diagonal and off-diagonal. (The situation here is analogous to the calculation of the quantum corrections to reflection in a normal billiard [9].) The off-diagonal corrections result from the Sieber–Richter (SR) [9, 13] pairs of trajectories. Such trajectories are exponentially close in the phase space (up to a time reversal), apart from a small region where one of them has a self-crossing and

the other has an anticrossing. Their actions differ by a small amount $\Delta\mathcal{S}(\varepsilon)$ depending on the crossing angle ε. Without the diagonality requirement $\Phi = 0$, a more general condition (12) should be used. If $\gamma_1 = \gamma_2$ has a crossing (anticrossing), it can be paired with $\gamma_1' = \gamma_2'$ which begins and ends exponentially close to $(\gamma_1)^{-1}$, but has an anticrossing (crossing). Their phase difference $\Phi = \pm l\Delta\mathcal{S}(\varepsilon_{\gamma_1})$ (see appendix A.1 for $l > 2$) is small compared to their actions. Hence, the momentum integration, as above, yields the SR correction to (5)

$$\langle \mathrm{Tr}[S(E)S^*(-E)]^l\rangle_{\mathrm{SR}} = 2\sum_{n,m=1}^{N}\sum_{\{\gamma(n,m)\}} |\mathcal{A}_\gamma|^2 \exp\left(\frac{\mathrm{i}}{\hbar}2lE\mathcal{T}_\gamma\right)\cos\left[\frac{l\Delta\mathcal{S}(\varepsilon_{\{\gamma\}})}{\hbar}\right], \tag{15}$$

where the index $\{\gamma\}$ runs over all self-crossings of the path γ. Performing the summation over the crossings by the standard procedure [9, 13–15], we arrive at the final result

$$\langle \mathrm{Tr}[S(E)S^*(-E)]^l\rangle_{\mathrm{SR}} = -\frac{1}{lN\mathcal{T}_{\mathrm{esc}}}\sum_{n,m=1}^{N}\sum_{\gamma(n,m)} |\mathcal{A}_\gamma|^2\mathcal{T}_\gamma \exp\left(\frac{\mathrm{i}}{\hbar}2lE\mathcal{T}_\gamma\right) \tag{16}$$

depending on the average escape time $\mathcal{T}_{\mathrm{esc}} = \pi\mathsf{A}/wv_F$, where v_F is the Fermi velocity (appendix B).

The diagonal quantum correction is

$$\langle \mathrm{Tr}[S(E)S^*(-E)]^l\rangle_{\mathrm{diag}} = \frac{1}{l}\sum_{n=1}^{N}\sum_{\gamma(n,n)} |\mathcal{A}_\gamma|^2 \exp\left(\frac{\mathrm{i}}{\hbar}2lE\mathcal{T}_\gamma\right). \tag{17}$$

For $l = 1$, it is readily derived using equation (2). Namely, in $\langle \mathrm{Tr}\, SS^*\rangle = \sum_{nm}\sum_{\gamma,\gamma'}\langle\cdots\rangle$ the terms with $n = m$ and $\gamma = \gamma'$ are considered. Since the actions of the *identical* paths cancel in the phase, these terms survive the averaging over k_F and yield the above result. Note that the terms with the *time-reversed* paths $\gamma = \gamma'^{-1}$ enter the classical part (5). In the case $l > 1$, the preceding integration procedure needs to be modified. This is done in appendix A.2. It is worth mentioning that both the SR and diagonal corrections are of the next order in N^{-1} to the classical contribution.

For the following calculation, it will be helpful to have the sums over the trajectories in (16) and (17) transformed into integrals over time. This can be achieved by using the sum rule for chaotic billiards [9]:

$$\sum_{\gamma(n,m)} |\mathcal{A}_\gamma|^2\delta(\mathcal{T} - \mathcal{T}_\gamma) \simeq N^{-1}P(\mathcal{T}), \tag{18}$$

where $P(\mathcal{T}) = (\mathcal{T}_{\mathrm{esc}})^{-1}\exp(-\mathcal{T}/\mathcal{T}_{\mathrm{esc}})$ is the survival probability. Adding the SR and diagonal contributions together, we obtain the total quantum correction:

$$\langle \mathrm{Tr}[S(E)S^*(-E)]^l\rangle_{\mathrm{quant}} = \frac{1}{l}\int_0^\infty \mathrm{d}\mathcal{T}\, P(\mathcal{T})\left(1 - \frac{\mathcal{T}}{\mathcal{T}_{\mathrm{esc}}}\right)\exp\left(\frac{\mathrm{i}}{\hbar}2lE\mathcal{T}\right). \tag{19}$$

2.3. Quantum correction to the density of states

The quantum correction to the DoS, originating from the SR and diagonal contributions,

$$\delta d(E) = \frac{2}{\pi\hbar}\int_0^\infty \mathrm{d}\mathcal{T}\, P(\mathcal{T})\mathcal{T}\left(1 - \frac{\mathcal{T}}{\mathcal{T}_{\mathrm{esc}}}\right)\ln\left(2\left|\cos\frac{E\mathcal{T}}{\hbar}\right|\right), \tag{20}$$

is found by substituting the corrections to the traces (19) in equation (1). In deriving (20), the sum over l was computed as follows:

$$\mathrm{Re}\sum_{l=1}^{\infty}\frac{(-1)^l}{l}\exp\left(\frac{\mathrm{i}}{\hbar}2lE\mathcal{T}\right) = -\mathrm{Re}\ln\left[1 + \exp\left(\frac{\mathrm{i}}{\hbar}2E\mathcal{T}\right)\right] = -\ln\left(2\left|\cos\frac{E\mathcal{T}}{\hbar}\right|\right). \tag{21}$$

Important conclusions can be drawn from (20) already in the limit $E/E_{\rm Th} \ll 1$, where $E_{\rm Th} = \hbar/2\mathcal{T}_{\rm esc}$ is the Thouless energy. In this case, one finds

$$\delta d(E) \approx -\frac{1}{\pi E_{\rm Th}}\left[\ln 2 - \left(\frac{3}{2}\frac{E}{E_{\rm Th}}\right)^2\right]. \tag{22}$$

We recall that the classical part of the DoS [4, 16]

$$d_{\rm cl}(E) = d_0 x^2 \frac{\cosh x}{\sinh^2 x}, \qquad x \equiv \frac{\pi E_{\rm Th}}{E}, \tag{23}$$

becomes exponentially small in this limit. Hence, equation (22) implies that the total DoS is *negative* at small energies. This unphysical result has two possible explanations: either there are other sources of quantum corrections not taken into account in the present work or the semiclassical theory becomes inapplicable near E_F, thereby reflecting the existence of the gap. Assuming the latter, we can roughly estimate the gap width E_g by setting $d_{\rm cl}(E_g) + \delta d(E_g) = 0$. This energy is weakly dependent on the channel number N and reads $E_g/E_{\rm Th} \approx 0.45, 0.34$ for $N = 10, 100$, respectively. These numbers are comparable with the results of the random-matrix theory [3] $E_g/E_{\rm Th} \approx 0.6$, as well as the full quantum calculations [4].

3. Conductance

In this section, we derive semiclassical formulae for the conductance G of a chaotic billiard having one normal (N) and one superconducting (S) lead. It was shown [6, 7] that $G = (4e^2/h)R_A$, where R_A is the Andreev-reflection coefficient defined in the introduction. It can be expressed [10] in terms of the electron transmission matrices $t_{\rm SN}$ and $t_{\rm NS}$ between the leads as

$$R_A = {\rm Tr}[t_{\rm SN} t_{\rm NS}^* (2 - t_{\rm SN} t_{\rm NS}^*)^{-1}]^2 \tag{24}$$

(it is assumed that $E = 0$). Expanding the denominators in the Taylor series, we obtain

$$R_A = \sum_{l,l'=1}^{\infty} 2^{-(l+l')}\, {\rm Tr}(t_{\rm SN} t_{\rm NS}^*)^{l+l'}, \tag{25}$$

which is a convenient starting point for the semiclassical treatment.

The semiclassical expressions for $t_{\rm SN}$ and $t_{\rm NS}$ are of the form (2) where the trajectories γ now connect the respective leads. The calculation of the traces in equation (25) (averaged over k_F) is completely analogous to that of the preceding section. For the classical contribution we find

$$R_{A,{\rm cl}} = \sum_{n=1}^{N_{\rm S}} \sum_{m=1}^{N_{\rm N}} \sum_{\gamma(n,m)} |\mathcal{A}_\gamma|^2 = T_{\rm cl}, \tag{26}$$

where $N_{\rm S,N}$ is the number of channels in the leads and $T_{\rm cl}$ is the classical transmission coefficient for electrons. It was taken into account that the classical traces are independent of $l + l'$ ($E = 0$) and that $\sum_{l,l'=1}^{\infty} 2^{-(l+l')} = 1$. This result supports the classical argument, according to which all trajectories that reach the superconducting lead will contribute to $R_{A,{\rm cl}}$. The quantum correction due to the SR pairs (there is no diagonal correction) becomes

$$R_{A,{\rm SR}} = T_{\rm SR} \sum_{l,l'=1}^{\infty} [(l + l')2^{l+l'}]^{-1} = T_{\rm SR} \ln 2, \tag{27}$$

where $T_{\rm SR} < 0$ is the standard SR correction to the electron transmission coefficient [9]. Thus, the weak-localization correction is smaller in an Andreev billiard than in the normal billiard of the same shape.

4. Summary and conclusions

We presented a new method which allows us to calculate traces of semiclassical scattering matrices in the Andreev billiards. The method was applied to determine the density of states and conductance in the chaotic cavities. The classical contribution to these quantities was found to be in agreement with the existing theories. The current framework made it possible to compute the quantum corrections to the classical results. We have shown that the weak-localization correction in the two-probe geometry is reduced, compared to the normal billiard of the same shape. In the closed cavity, the quantum corrections make the density of states negative within a small distance (of the order of the Thouless energy) from the Fermi level. If this property is a signature of the gap in the density of states discovered by other methods, it will be important to understand the failure of the semiclassical theory close to the Fermi energy. Alternatively, other, so far unknown, types of quantum corrections could compensate the negative value.

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Appendix A. Derivations for arbitrary *l*

A.1. Classical contribution

We start with the generalization of integral (8)

$$\mathrm{Tr}[S(E)S^*(-E)]^l = \left(\frac{w}{\pi\hbar}\right)^{2l} \int_{-\hbar k_F}^{\hbar k_F} \mathrm{d}p_1\,\mathrm{d}p_1' \cdots \mathrm{d}p_l\,\mathrm{d}p_l' \times \sum_{\substack{\gamma_1,\gamma_1',\\ \cdots\\ \gamma_l,\gamma_l'}} \mathcal{A}_{\gamma_1}\mathcal{A}^*_{\gamma_1'} \cdots \mathcal{A}_{\gamma_l}\mathcal{A}^*_{\gamma_l'} \exp\left(\frac{\mathrm{i}}{\hbar}\Phi\right) \exp\left(\frac{\mathrm{i}}{\hbar}2lE\overline{\mathcal{T}}\right), \tag{A.1}$$

where the paths, in terms of their initial and final momenta, are $\gamma_j(p_j \leftarrow -p_j')$ and $\gamma_j'(p_j' \leftarrow -p_{j+1})$ $(j = 1, \ldots, l;\ l+1 \equiv 1)$, $\Phi = \sum_{j=1}^{l}\left(\mathcal{S}_{\gamma_j} - \mathcal{S}_{\gamma_j'}\right)$ and $\overline{\mathcal{T}} = (2l)^{-1}\sum_{j=1}^{l}\left(\mathcal{T}_{\gamma_j} + \mathcal{T}_{\gamma_j'}\right)$. As in (9), we transform to the new variables

$$\begin{pmatrix} a_1 \\ \vdots \\ a_{l-1} \\ b \end{pmatrix} = C \begin{pmatrix} p_1 \\ \vdots \\ p_l \end{pmatrix} \qquad \text{and} \qquad \begin{pmatrix} a_1' \\ \vdots \\ a_{l-1}' \\ b' \end{pmatrix} = C \begin{pmatrix} p_1' \\ \vdots \\ p_l' \end{pmatrix} \tag{A.2}$$

in such a way that b and b' are within the manifold

$$\begin{cases} p_1 = \cdots = p_l \equiv \overline{p} \\ p_1' = \cdots = p_l' \equiv \overline{p}' \end{cases} \quad (|p_i|, |p_i'| \leqslant k_F), \tag{A.3}$$

while a_i and a'_i are transverse to it. This means that C is an orthogonal matrix which has the property $\sum_{j=1}^{l} C_{ij} = 0$ $(i = 1, \ldots, l-1)$. It is convenient to choose this matrix in the form

$$C = \begin{bmatrix} \frac{1}{\sqrt{1\cdot 2}}(1, & -1, & 0, & 0, & 0, & \ldots, & 0, & 0) \\ \frac{1}{\sqrt{2\cdot 3}}(1, & 1, & -2, & 0, & 0, & \ldots, & 0, & 0) \\ \frac{1}{\sqrt{3\cdot 4}}(1, & 1, & 1, & -3, & 0, & \ldots, & 0, & 0) \\ & & & & \ldots & & & \\ \frac{1}{\sqrt{(l-1)l}}(1, & 1, & 1, & 1, & 1, & \ldots, & 1, & -(l-1)) \\ \frac{1}{\sqrt{l}}(1, & 1, & 1, & 1, & 1, & \ldots, & 1, & 1) \end{bmatrix}, \tag{A.4}$$

where the rows are multiplied by the factors in front of them.

The derivatives of the phase function

$$\frac{\partial \Phi}{\partial a_k} = \sum_{j=1}^{l} \left(-y^f_{\gamma_j} C^T_{jk} + y^i_{\gamma'_j} C^T_{j+1,k}\right), \tag{A.5}$$

and similar for $\partial\Phi/\partial a'_k$, vanish if $\gamma_1 = \cdots = \gamma_l \equiv \overline{\gamma}$ and $\gamma'_1 = \cdots = \gamma'_l \equiv \overline{\gamma}'$. In the diagonal approximation, we have $\Phi = 0$ and $\overline{\gamma} = (\overline{\gamma}')^{-1}$. In the SR quantum correction, $\overline{\gamma}$ and $(\overline{\gamma}')^{-1}$ form the SR pair, and the phase is $\Phi = \pm l\,\Delta\mathcal{S}(\varepsilon_{\overline{\gamma}})$.

We proceed in the diagonal approximation. The non-vanishing second derivatives of Φ at the SP point are

$$\left.\frac{\partial^2 \Phi}{\partial a_i \partial a'_k}\right|_{a_j = a'_j = 0} = -\frac{\partial^2 \mathcal{S}_{\overline{\gamma}}(\overline{p}, -\overline{p}')}{\partial \overline{p}\,\partial(-\overline{p}')} D_{ik}, \tag{A.6}$$

where we introduced the $(l-1)\times(l-1)$ matrix $D_{ik} \equiv \delta_{ik} - \sum_{j=1}^{l} C_{i,j+1} C^T_{jk}$. Equation (A.4) yields an explicit expression $D_{ik} = \widetilde{D}_{ik}/\sqrt{i(i+1)k(k+1)}$ in terms of the matrix

$$\widetilde{D} = \begin{pmatrix} 1\cdot 2+1 & -1\cdot 3 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 1 & 2\cdot 3+1 & -2\cdot 4 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 1 & 1 & 3\cdot 4+1 & -3\cdot 5 & 0 & \cdots & 0 & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 1 & 1 & 1 & 1 & 1 & \cdots & 1 & (l-2)(l-1)+1 & -(l-2)l \\ l & l & l & l & l & \cdots & l & l & l^2 \end{pmatrix}. \tag{A.7}$$

Its determinant $\det \widetilde{D} = (l!)^2$ can be computed by adding the first column to the second column, then adding the resulting second column to the third column and so on. Hence, the Hessian of Φ is given by

$$\det \Phi'' \equiv \begin{vmatrix} \left(\frac{\partial^2\Phi}{\partial a_i \partial a_k}\right) & \left(\frac{\partial^2\Phi}{\partial a_i \partial a'_k}\right) \\ \left(\frac{\partial^2\Phi}{\partial a'_i \partial a_k}\right) & \left(\frac{\partial^2\Phi}{\partial a'_i \partial a'_k}\right) \end{vmatrix} = \left[\frac{\partial^2 \mathcal{S}_{\overline{\gamma}}(\overline{p}, -\overline{p}')}{\partial \overline{p}\,\partial(-\overline{p}')}\right]^{2(l-1)} l^2. \tag{A.8}$$

To complete the SP integration,

$$\int \left(\prod_{j=1}^{l} \mathrm{d}a_j\, \mathrm{d}a'_j\right) \exp\left(\frac{\mathrm{i}}{\hbar}\Phi\right)(\cdots) \approx \frac{(2\pi\hbar)^{l-1}}{|\det \Phi''|^{1/2}} \exp\left(\frac{\mathrm{i}}{\hbar}\Phi + \mathrm{i}\frac{\pi}{4}\,\mathrm{sgn}\,\Phi''\right)(\cdots), \tag{A.9}$$

we find the difference of the number of positive and negative eigenvalues of Φ'', $\mathrm{sgn}\,\Phi'' = 0$. This can be shown as follows: if an eigenvector of $\left(\begin{smallmatrix} 0 & A \\ B & 0 \end{smallmatrix}\right)$ with an eigenvalue λ is $\left(\begin{smallmatrix} \alpha \\ \beta \end{smallmatrix}\right)$, then $\left(\begin{smallmatrix} \alpha \\ -\beta \end{smallmatrix}\right)$

is an eigenvector with the eigenvalue $-\lambda$ (here A and B are the square matrices and α and β are the columns of equal size). After the last two integrations over $\mathrm{d}b\,\mathrm{d}b'$ along the manifold (A.3) we end up with equation (5).

A.2. Diagonal quantum corrections

Let us repeat the SP integration over $\prod_{j=1}^{l}\mathrm{d}a_j\,\mathrm{d}a'_j$ in appendix A.1 with the exception that now $\overline{\gamma}=\overline{\gamma}'$, instead of $\overline{\gamma}=(\overline{\gamma}')^{-1}$, is taken at the stationary point. This choice is compatible with the diagonality condition $\Phi=0$ and is possible on the manifold $\overline{p}=\overline{p}'$. It is convenient to perform the remaining integrations over $\mathrm{d}b\,\mathrm{d}b'$ in the transformed coordinates $b_\pm=l^{\mp1/2}(b\pm b')/\sqrt{2}$ such that $\Phi=0$ is fulfilled on the line $b_-=0$. The subsequent averaging over k_F is expected to pick up the contribution of the neighbourhood of this line (diagonal approximation). Therefore, we can expand $\Phi\approx(\partial\Phi/\partial b_-)b_-$, where $\partial\Phi/\partial b_-=\left(y^i_{\overline{\gamma}}-y^f_{\overline{\gamma}}\right)\big/\sqrt{2}$. This leads to the result

$$\langle\mathrm{Tr}[S(E)S^*(-E)]^l\rangle_{\mathrm{diag}}\approx\frac{1}{l}\left(\frac{w}{\pi\hbar}\right)^2\left\langle\int_{-\hbar k_F}^{\hbar k_F}\mathrm{d}b_+\sum_{\overline{\gamma}(\overline{p}\leftarrow\mp\overline{p})}|\mathcal{A}_{\overline{\gamma}}|^2\exp\left(\frac{\mathrm{i}}{\hbar}2lE\mathcal{T}_{\overline{\gamma}}\right)\right.$$
$$\left.\times\int\mathrm{d}b_-\exp\left(\frac{\mathrm{i}}{\hbar}\frac{\pm y^i_{\overline{\gamma}}-y^f_{\overline{\gamma}}}{\sqrt{2}}b_-\right)\right\rangle. \tag{A.10}$$

Note that this formula includes two classes of trajectories, $\overline{\gamma}(\overline{p}\leftarrow-\overline{p})$ and $\overline{\gamma}(\overline{p}\leftarrow\overline{p})$, and, correspondingly, two signs of $y^i_{\overline{\gamma}}$ in the second exponent. The latter class is taken into account if one starts from equation (A.1) with $\gamma_j(p_j\leftarrow p'_j)$ and $\gamma'_j(p'_j\leftarrow p_{j+1})$.

One can avoid explicit calculation of equation (A.10) by comparing it with the result (17) for $l=1$, which was derived independently. It is then quite obvious that (17) is valid for arbitrary l.

Appendix B. Summation over the Sieber–Richter pairs

The purpose of this section is to fill in the steps between equations (15) and (16). For a trajectory γ, the average number of self-crossings with the crossing angle between ε and $\varepsilon+\mathrm{d}\varepsilon$ is [9]

$$P_X(\varepsilon;\mathcal{T}_\gamma)\,\mathrm{d}\varepsilon\approx\frac{\mathcal{T}_\gamma^2v_F^2}{\pi\mathsf{A}}\sin\varepsilon\left[\frac{1}{2}-2\frac{\mathcal{T}_{\min}(\varepsilon)}{\mathcal{T}_\gamma}\right]\mathrm{d}\varepsilon, \tag{B.1}$$

where $\mathcal{T}_{\min}(\varepsilon)$ is the size of the crossing region (logarithmically dependent on ε). We took into account the correction put forward in [15], according to which the $\mathcal{T}_{\min}(\varepsilon)$ contribution in (B.1) is twice as large as was previously suggested in [9]. The terms of higher order in $\mathcal{T}_{\min}(\varepsilon)/\mathcal{T}_\gamma$ are neglected. It is important to keep the contribution proportional to $\mathcal{T}_{\min}(\varepsilon)$, since the subsequent integration over ε would eliminate the leading term [13].

With the help of (B.1), the sum over the self-crossings in (15) can be reduced to the sum over the paths as $\sum_{\{\gamma(n,m)\}}(\cdots)\to\int\mathrm{d}\varepsilon\sum_{\gamma(n,m;\varepsilon)}P_X(\varepsilon;\mathcal{T}_\gamma)(\cdots)$, where the index $\gamma(n,m;\varepsilon)$ runs over all paths having a self-crossing of angle ε. Let us, for a moment, transform the latter sum to an integral using the sum rule (18). It was noted by the authors of [15] that the sum rule has a correction linear in $\mathcal{T}_{\min}(\varepsilon)$. It can be obtained by shifting $\mathcal{T}\mapsto\mathcal{T}-\mathcal{T}_{\min}(\varepsilon)$ in the right-hand side of (18). Thus, there are two contributions of the first order in $\mathcal{T}_{\min}(\varepsilon)$: the one coming from the leading-order term in (B.1) and the first-order correction to the sum rule and the other resulting from the $\mathcal{T}_{\min}(\varepsilon)$ term in (B.1) and the uncorrected sum rule. Integrating

over $\mathcal{T}$ explicitly, one can show that the former contribution is two times smaller than the latter and has the opposite sign.

The preceding argument allows, in effect, us to consider the half of the first-order term in (B.1) and transform $\sum_{\{\gamma(n,m)\}}(\cdots) \to \sum_{\gamma(n,m)} \int \mathrm{d}\varepsilon\, P_X(\varepsilon; \mathcal{T}_\gamma)(\cdots)$. The ε integral was computed in [13] and reads

$$\frac{v_F^2}{\pi \mathsf{A}} \int_0^\pi \mathrm{d}\varepsilon \cos\left[\frac{l\Delta\mathcal{S}(\varepsilon)}{\hbar}\right] \sin(\varepsilon)\mathcal{T}_{\min}(\varepsilon) \approx \frac{1}{2Nl\mathcal{T}_{\mathrm{esc}}}. \tag{B.2}$$

Then equation (16) would follow.

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