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The energy spectrum and the persistent current in multi-channel rings

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Abstract. In this paper the correlation in the energy spectrum and the persistent current of multi-channel disordered rings threaded by an Aharonov–Bohm magnetic flux are studied. The correlations of the persistent currents are found to be not as strong as those in single-channel disordered rings. The results show that, for a tight-binding model with N sites on the circumference and M sites on the cross-sectional plane, there are at least $N-1$ zero crossings of the single-level currents, and at least $N-2$ zero crossings of the total currents at zero and high temperatures.

1. Introduction

The persistent current in conducting rings threaded by Aharonov–Bohm magnetic flux has been discussed ever since the discovery of the Aharonov–Bohm effect in superconducting rings. Since the work by Büttiker, Imry, and Landauer [1] in 1983, interest in this area has been renewed. Theoretical work [2–6] predicted, and subsequent experimental work [7–9] confirmed, the existence of persistent current in the rings. Results on persistent current of a ring also give us information on the energy spectrum, since the current can be calculated from the derivative of the eigenenergy with respect to the magnetic flux. Previously, the correlation in the energy spectrum of single-channel rings has been discussed by Cheung and Riedel [10]. They proved that within a non-interacting model with arbitrary disorder, the single-level current changes sign from level to level, and the total current alternates its sign as the number of filled levels increases by one. Another way of putting this is that, for a tight-binding model of single-channel rings which has N sites, the single-level current changes sign $N-1$ times, while the ground-state total current changes sign $N-2$ times as the number of electrons increases. We define the zero crossings of the single-level current as the energies at which the current of the level just below and the current of the level just above are of the opposite sign. We define the zero crossings of the total current as the chemical potentials [11] at which the total current changes sign. Thus for the above rings, there are $N-1$ zero crossings for the single-level current, and $N-2$ zero crossings for the total current.

In this article we extend the above results to multi-channel rings. Previously Cheung, Riedel, and Gefen [4] have shown that in the diffusive regime the single-level currents of energy levels within the energy range $E_c \sim \Delta l/L$ are correlated, where Δ is the energy spacing for one channel, l is the mean free path, and L is the size of the ring in units of the

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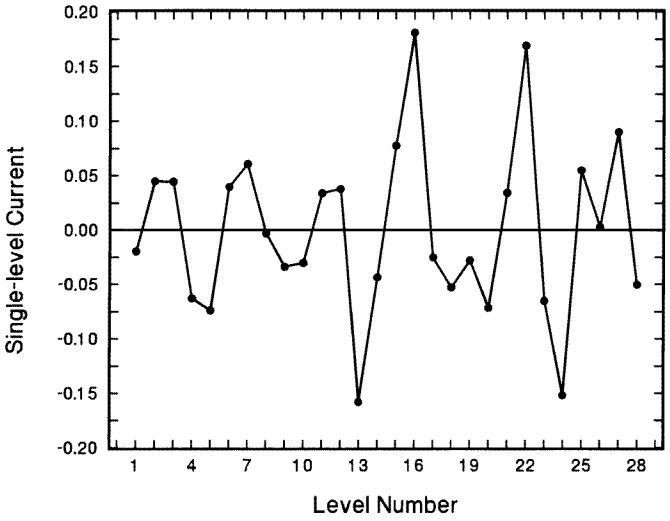

Figure 1. The numerical result for single-level currents on a multi-channel ring with seven sites along its circumference, four sites on its transverse direction (number of channels = 4), and disorder $W = 8$. The currents are normalized so that the maximum single-level current of a pure ring is 1. The levels are arranged in order of increasing energy.

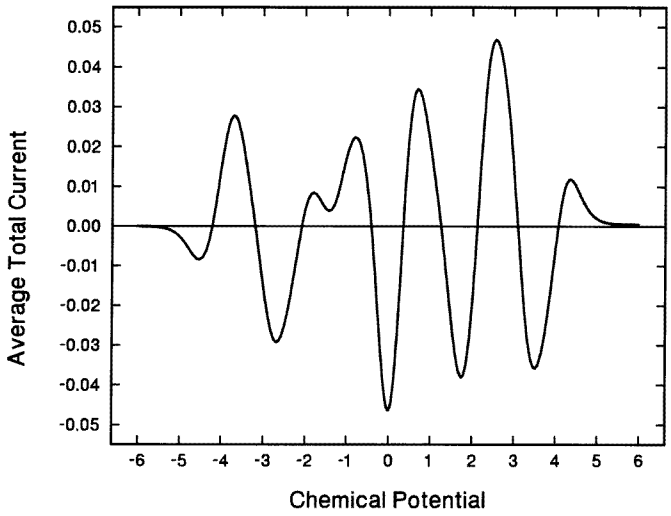

Figure 2. The numerical result for the total current of the same ring as in figure 1, at temperature $k_BT = 0.2V$, as a function of the chemical potential. The chemical potential is also measured in units of the tight-binding hopping matrix element V.

lattice spacing. This means that, in the diffusive regime, the single-level current changes sign roughly l times, in the ballistic regime the single-level current changes sign roughly L times, and in the localized regime the sign of the single-level current is almost random from level to level. The result of Cheung, Riedel, and Gefen [4] gives no hint as to the behaviour of the total current. In addition, this result is for the average behaviour only. There has been no result obtained that is applicable for every ring. Figures 1 and 2 show some of our

numerical results. They show that the single-level and the total persistent currents change sign many times. However, the pattern is less regular than that for single-channel rings. These results must be known to researchers in the field, but there have not been specific discussions of them.

In the sections below, the following points are discussed, and proofs given. (1) How often do the single-level and total persistent currents change sign? (2) How do the disorder and thermal fluctuation affect the sign changes for the single-level and total persistent currents? The discussion is based on a ring described by a non-interacting tight-binding model with N sites on the circumference and M sites on the cross-sectional plane. It is proved that for arbitrary disorder, and at both zero and high temperatures, the single-level and total persistent currents have at least $N-1$ and $N-2$ zero crossings respectively.

2. The transfer-matrix-matching method and the moment conditions

Consider two- or higher-dimensional (multi-channel) rings having of N sites on the circumferences and M sites on the cross-sectional plane. The position along the circumference is described by an integer j that take values from 1 to N, and the position on the cross-sectional area is described by an integer k (k') which can take values from 1 to M. k and k' are nearest-neighbouring sites on the cross-sectional plane. The tight-binding Hamiltonian of the electrons on such rings is

$$H = -V\sum_{j,k}\left[a^{+}_{j,k}a_{j+1,k} + a^{+}_{j+1,k}a_{j,k} + \sum_{k'}(a^{+}_{j,k}a_{j,k'} + a^{+}_{j,k'}a_{j,k})\right] + \sum_{j,k}\varepsilon_{j,k}a^{+}_{j,k}a_{j,k} \tag{1}$$

where $a^{+}_{j,k}$ and $a_{j,k}$ are the creation and annihilation operators at site (j,k), V is the hopping matrix element, and $\varepsilon_{j,k}$ is the potential at site (j,k) and is assigned randomly. The presence of an Aharonov–Bohm flux through a ring is equivalent to imposing a phase-shifted boundary condition on the wavefunctions.

In the following, the transfer-matrix-matching method of finding the eigenenergies and eigenfunctions is described. The transfer-matrix-matching method is essentially the 'shooting' method of solving the time-independent Schrödinger equation. Let the collection of sites with the same j be referred to as the jth column. In this way each cross-sectional plane of the ring is called a column, and there are N of them. The idea is to start with a trial eigenenergy E, and a trial eigenfunction for the first two columns (sites with $j = 1$ and 2). This is equivalent to specifying the wavefunction and its derivative on a cross-sectional plane. Then by enforcing the time-independent Schrödinger equation on the second column, the eigenfunction on the third column can be calculated. The relation between the eigenfunctions for different columns is linear, and can be written in terms of a matrix called the transfer matrix [12]. By repeating this process, the eigenfunctions can be determined over the whole ring. Each time one more column is involved, one more matrix multiplies the existing matrix to form a combined transfer matrix, until one has gone around the ring once. By imposing the appropriate boundary conditions, we have

$$\begin{pmatrix}\psi_{N+1}\\ \psi_{N+2}\end{pmatrix} = T\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix} = \mathrm{e}^{\mathrm{i}\,2\pi\Phi/\Phi_0}\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix} \tag{2}$$

where ψ_j is the eigenfunction for column j, and T is the transfer matrix for going around the ring once. Φ and Φ_0 denote the applied magnetic flux and the flux quantum ($=hc/e$ in gaussian units) respectively. For non-trivial solutions to equation (2), the eigenenergies satisfy the following characteristic equation:

$$\mathrm{Det}(T - \mathrm{e}^{\mathrm{i}\,2\pi\Phi/\Phi_0}) = 0. \tag{3}$$

From the construction, we note that the left-hand side of equation (3) is a polynomial in E of order NM. Thus there are altogether NM eigenenergies E_i, and their corresponding eigenfunctions can be found for any given magnetic flux Φ. The determinant in equation (3) can be rewritten in terms of the sums of the principle minors [13] of T. After simplification, equation (3) becomes

$$g(E,\Phi) \equiv 2\cos\left(\frac{2M\pi\Phi}{\Phi_0}\right) + 2\sum_{p=1}^{M-1}\left[(-1)^{M-p}\cos\left(\frac{2p\pi\Phi}{\Phi_0}\right)\mathrm{Tr}_{M-p}\right] + (-1)^M\mathrm{Tr}_M = 0 \tag{4}$$

where $g(E,\Phi)$ is a newly defined function introduced to simplify the notation, and Tr_j is the sum of the principal minors of T of order j. For example, Tr_1 is the trace of T. Due to probability conservation and time-reversal symmetry, $\mathrm{Tr}_{2M} = \mathrm{Det}(T) = 1$ and $\mathrm{Tr}_j = \mathrm{Tr}_{2M-j}$, where $j = 1, 2, \ldots, M$. Since $g(E,\Phi)$ is also a polynomial of order NM in E, it can be rewritten as

$$g(E,\Phi) \propto \prod_{i=1}^{NM}[E - E_i(\Phi)]. \tag{5}$$

In equation (4), one can check that Tr_M is a polynomial of degree NM in E, and that all other Tr_j are of maximum degree $N(M-1)$ in E. That is, when $g(E,\Phi)$ is expressed as a polynomial, the coefficients of $E^{N(M-1)+1}, E^{N(M-1)+2}, \ldots, E^{NM}$ are flux independent. This fact can lead to a proof of the 'moment conditions' that was first pointed out by Thouless [14], who stated that the first $(N-1)$th moments of the energy spectrum are flux independent. Expressed in mathematical form, this is

$$\sum_{i=1}^{NM} E_i^j(\Phi) = \text{flux-independent quantities} \tag{6}$$

where $j = 1, 2, \ldots, N-1$. A proof of the moment conditions had been given by Cheung and Riedel [10].

From the above moment conditions, one can deduce that the rigidity of the energy spectrum is less than that in single-channel rings [10]. The reason for this is that the N eigenenergies of the single-channel rings have to satisfy $N-1$ moment conditions, whereas the NM eigenenergies of the multi-channel rings have to satisfy only $N-1$ moment conditions. As a consequence, the degrees of freedom of the eigenenergies increase and the number of zero crossings of the current can no longer be obtained exactly. In the following sections, the zero crossings of the currents will be analysed.

3. Zero crossings of the single-level currents at zero temperature

By applying the well known current formula $I_i = -c\,\partial E_i/\partial\Phi$ to the moment conditions, one can obtain a system of homogeneous linear equations relating the single-level currents of different levels:

$$\sum_{i=1}^{NM} E_i^j(\Phi) I_i = 0 \tag{7}$$

where $j = 0, 1, 2, \ldots, N-2$. Equation (7) is a useful starting point for deriving the minimum number of zero crossings of single-level currents. The derivation is presented here. First arrange the eigenenergies in ascending order. Let R be the number of different zero crossings of the single-level currents, and suppose $R \leqslant N-2$. The zero crossings

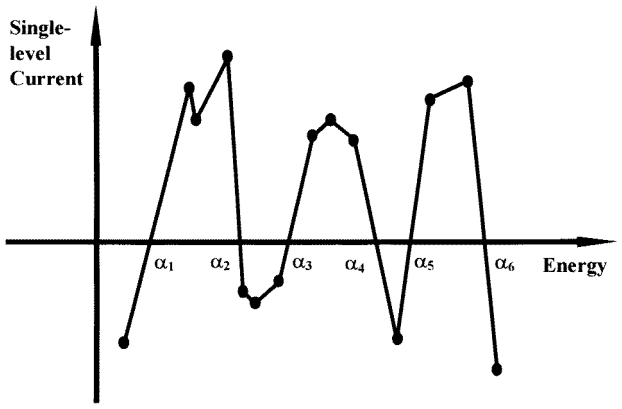

Figure 3. A schematic plot of the single-level current against energy in a multi-channel ring with $N = 7$ and $M = 2$. The levels with energy E and current I are represented by dots on the graph. $\alpha_1, \alpha_2, \ldots, \alpha_6$ are zero crossings and not energy levels in the spectrum. In this example, there are in total six zero crossings of the single-level currents.

are labelled as $\alpha_1, \alpha_2, \ldots, \alpha_R$ on the energy axis. An example is shown in figure 3. Now consider the expression $\sum_{i=1}^{NM} f(E_i)I_i$ where $f(E) = \prod_{j=1}^{R}(E - \alpha_j)$. From the construction, $f(E_i)I_i$ is either completely positive or negative for all i, and hence its sum cannot be zero. On the other hand, we can analyse the same expression in another way—that is, by expanding $f(E)$ as a polynomial in E. In this way, one obtains $\sum_{i=1}^{NM} f(E_i)I_i = 0$ after using equation (7), and this result contradicts the above result that $\sum_{i=1}^{NM} f(E_i)I_i \neq 0$. To avoid the contradiction, there must be at least $N - 1$ zero crossings of the single-level currents. An alternative method is also given in the appendix.

4. Zero crossings of the total currents at zero temperature

In a previous paper [10], it has been proven that the total current changes sign every time that one more level is filled, except when the first or last level is filled. Thus there are $N - 2$ zero crossings for a single-channel ring with N sites on its circumference. We now focus on the multi-channel rings. The analysis follows that for the single-channel ring [10], with extra complications.

Recall that the eigenenergies $E_i(\Phi)$ are roots of the equation $g(E, \Phi) = 0$ for a given magnetic flux Φ. Accordingly, if Φ is changed by an infinitesimal amount $\mathrm{d}\Phi$, and hence E_i changes by an infinitesimal amount $\mathrm{d}E$, $g(E, \Phi)$ should remain at zero. That is to say

$$\mathrm{d}g = \frac{\partial g}{\partial E}\,\mathrm{d}E + \frac{\partial g}{\partial \Phi}\,\mathrm{d}\Phi = 0$$

and hence the current can be obtained from

$$I_i = -c\frac{\mathrm{d}E_i}{\mathrm{d}\Phi} = c\frac{\partial g}{\partial \Phi}\Big/\frac{\partial g}{\partial E}\bigg|_{E=E_i}. \tag{8}$$

Refer to the analysis in the last section: $g(E, \Phi)$ is a polynomial of degree NM in E, and the coefficients of $E^{N(M-1)+1}, E^{N(M-1)+2}, \ldots, E^{NM}$ are flux independent. Consequently, $\partial g/\partial \Phi$ is a polynomial of order $N(M-1)$. Let us denote the zeros of $\partial g/\partial \Phi$ by $e_m(\Phi)$, where $m = 1, 2, \ldots, N(M-1)$. Using equations (5) and (8), the single-level current I_n for

a particular level n can be rewritten as

$$I_n \propto \prod_{m=1}^{N(M-1)} [E_n(\Phi) - e_m(\Phi)] \Big/ \prod_{m=1}^{NM}{}' [E_n(\Phi) - E_m(\Phi)]$$
$$= \frac{1}{2\pi \mathrm{i}} \oint_{\mathrm{C}_{E_n}} \left(\prod_{m=1}^{N(M-1)} [E - e_m(\Phi)] \Big/ \prod_{m=1}^{NM} [E - E_m(\Phi)] \right) \mathrm{d}E$$
$$\equiv \frac{1}{2\pi \mathrm{i}} \oint_{\mathrm{C}_{E_n}} h(E, \Phi)\ \mathrm{d}E \tag{9}$$

where $h(E, \Phi)$ denotes the integrand of the integral. The above integration is over a closed contour C_{E_n} enclosing the pole at E_n. By choosing the contour of integration such that it encloses the lowest n eigenenergies, the total current of the first n levels can be expressed as

$$I_{total} \propto \frac{1}{2\pi \mathrm{i}} \oint_{\mathrm{C}} h(E, \Phi)\ \mathrm{d}E. \tag{10}$$

Equation (10) is a convenient starting point for deriving the minimum number of zero crossings of the total current. The crucial step in the derivation is to choose suitable contours of integration on the complex plane that allow the sign of the total current to be determined. In reality one needs a contour such that the integrand is purely real and does not change sign along the whole contour. If we rewrite the integrand as $|h(E, \Phi)|\mathrm{e}^{\mathrm{i}\theta}$, and restrict θ to taking only the values $\pm l\pi$ where l is any integer, some lines on the complex plane can be defined. On any one of these lines, the integrand will have a definite sign. In the following we will analyse these lines.

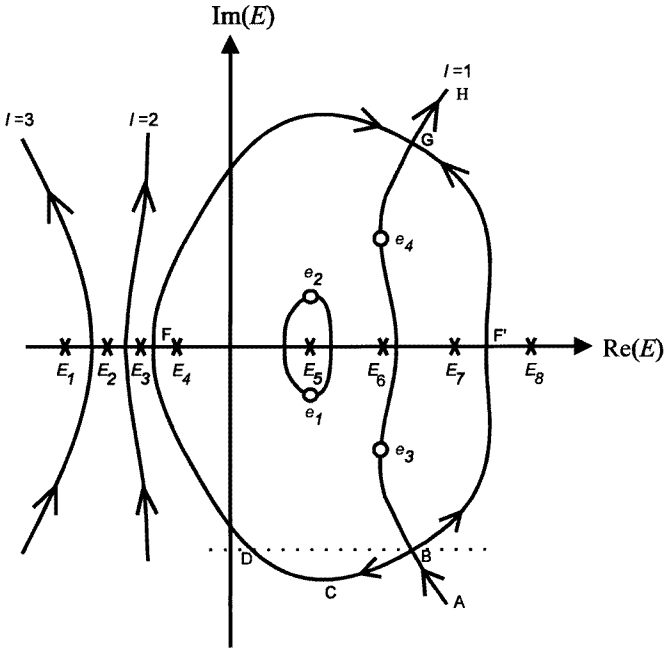

Figure 4. A schematic plot of the contours in equation (10) on the complex E-plane, with $N = 4$, $M = 2$. $\times$ and $\bigcirc$ represent the poles and zeros respectively.

Let us first look at the regions that are far away from the origin on the complex plane, and exclude the real axis. One sees that there are NM poles and $N(M-1)$ zeros in the integrand. Thus, in the regions concerned, one can easily see that there are exactly $N-1$ lines defined by $\theta = l\pi$, where l is an integer in the range from 1 to $N-1$. In the regions that are close to the poles and zeros of the integrand, these lines may acquire a complicated structure (see, for example, figure 4). Since the integrand is an analytic function, there cannot be any local maxima or minima in the open half-planes. This means that if one traces along any one of the $N-1$ lines from infinity in the lower half-plane, the sign of the integrand remains unchanged, and the absolute value of the integrand will increase from zero. At places where the line branches out, such as point B in figure 4, one can always choose such a path that the absolute value of the integrand keeps on increasing, until one reaches the real axis (for example, line BF′ in figure 4). Once the real axis has been crossed and the upper half-plane entered, one can choose a line that is mirror symmetric to that in the lower half-plane. In this way one has $N-1$ lines that start from infinity on the lower half-plane and go to infinity on the upper half-plane. Suppose that we choose any one of these lines as the integration contour in equation (10), and that the integration contours are closed at infinity, enclosing all of the eigenenergies to the left of the line; one can easily see that:

(1) the integration along the contour at infinity contributes nothing;

(2) when tracing upward along the line from infinity on the lower half-plane, the contribution to the imaginary part of the integral is of the same sign as that of the integrand; and

(3) occasionally the line may have to change its direction from upward to downward, before eventually turning upward again. One can see that the contribution to the imaginary part of the integral from such a section would change sign. However, this opposite contribution will be more than compensated by the section either just before or just after the section in question. For example, the contribution from section BC in figure 4 is of the opposite sign to that from section CD. However, the contribution from section CD will more than compensate the contribution from the section BC (since the absolute value of the integrand will be monotonically increasing as one traces along BCDF). So ABFGH is also a valid contour.

Along such a line, one can see that the imaginary part of the integral is of a definite sign [15], given by $(-1)^l$. This is the sign of the total current of the first n levels. Since there are $N-1$ lines regardless of the degree of disorder, we see that there are at least $N-2$ zero crossings [16].

5. Zero crossings of the total current at high temperatures

In this section we discuss the effects of thermal fluctuation on the zero crossings of the total average current. We consider the system within the grand-canonical ensemble [11]. In this way the occupation probability of each level is given by the Fermi–Dirac function. It would be interesting to know whether the correlation in the current would be weakened by thermal fluctuation.

Starting from equation (9) for the single-level current, the currents from all of the levels are summed using the Fermi–Dirac function. In this way the average total current can be written as

$$I_{total}(T) \propto \frac{1}{2\pi \mathrm{i}} \oint \frac{h(E,\Phi)}{\exp((E-\mu)/k_B T)+1}\,\mathrm{d}E \tag{11}$$

where T, μ, and k_B represent the temperature, chemical potential, and the Boltzmann factor respectively. The integration is from $-\infty$ to $+\infty$ just below the real axis, and from $+\infty$ to $-\infty$ just above the real axis. In this way all of the levels are counted. Since the Fermi–Dirac function is present, the contour below and above the real axis can be deformed to include all of the poles of the Fermi–Dirac function. The result is

$$I_{total}(T) \propto \sum_{\text{odd}\, m} h(\mu + \mathrm{i}m\pi k_B T, \Phi). \tag{12}$$

At high temperatures (i.e. $k_B T \gg$ energy spacing), the contributions from the $m = \pm 1$ terms dominate. Thus the average total current is twice the real part of the function $h(\mu + \mathrm{i}\pi k_B T, \Phi)$. From the analysis in the last section, one sees that θ changes from 0 to $N\pi$ as one moves in an anticlockwise fashion along a big circle in the upper half of the complex E-plane. This means that if the temperature is fixed at a high value, and the chemical potential μ is allowed to vary from $-\infty$ to $+\infty$, the average total current must have at least $N-2$ zero crossings [17]. The above calculations assume the grand-canonical ensemble. Similar results are obtained in numerical simulations assuming the canonical ensemble.

6. Discussion

We have proved that at both zero temperature and at high temperatures, there are at least $N-2$ zero crossings of the total current. At intermediate temperatures the situation for the number of zero crossings is still unclear. We conjecture that the number of zero crossings of the total currents at finite temperatures would be at least $N-2$ too, since (i) this would be consistent with the result at zero temperature and at high temperatures, and (ii) results with fewer zero crossings at intermediate temperatures have never been obtained in our numerical work.

It should be emphasized that, for multi-channel rings, the minimum number of zero crossings of the total current is the same as that for single-channel rings (i.e. $N-2$). This lowest bound is independent of the number of channels. From this result, the total current for multi-channel rings is not expected to change sign every time an extra electron is added. Instead, it would change sign if roughly M more electrons were added. This strong correlation between the currents occurs regardless of the degree of disorder of the system, and does not seem to depend on thermal fluctuation over the whole temperature range.

Acknowledgments

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Appendix

There is an alternative method for looking at the number of zero crossings of the single-level currents starting from the second expression of equation (9). As n increases, the denominator changes sign precisely $NM-1$ times, while the numerator changes sign only at most $N(M-1)$ times. So the number of sign changes of I_n as n goes from 1 to NM is at least $NM-1-N(M-1) = N-1$. This result is the same as what we have concluded—that there are at least $N-1$ zero crossings for the single-level currents.

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[14] The 'moment conditions' were first stated by D J Thouless. See reference [10] for details.
[15] The real part of the integral is zero, since both the integrand and the contour are mirror symmetric about the real axis.
[16] If one chooses the line ABe_3e_4GH as the integration contour, the integrand changes sign when passing across the zeros e_3 and e_4, and thus no definite conclusion can be drawn as to the sign of the total current.
[17] For extremely high temperatures—that is, when T is much greater than the imaginary part of all of the zeros e_m in $h(E, \Phi)$—there are exactly $N - 2$ zero crossings.