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# Enhancement of persistent current in metal rings by correlated disorder

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**Abstract**
We study analytically the effect of a correlated random potential on the persistent current in a one-dimensional ring threaded by a magnetic flux $\phi$, using an Anderson tight-binding model. In our model, the system of $N = 2M$ atomic sites of the ring is assumed to be partitioned into $M$ pairs of nearest-neighbour sites (dimers). While the individual atomic site energies are assumed to be identically distributed Gaussian variables with autocorrelation parameter $\varepsilon_0^2$, the dimer site energies are chosen to be correlated with a Gaussian strength $\alpha^2 < \varepsilon_0^2$. For this system we obtain the exact flux-dependent energy levels to second order in the random site energies, using an earlier exact transfer matrix perturbation theory. These results are used to study the mean persistent current generated by $N_e \leqslant N$ spinless electrons occupying the $N_e$ lowest levels of the flux-dependent energy band at zero temperature. Detailed analyses are carried out in the case of low filling of the energy band ($1 \ll N_e \ll N$) and for a half-filled band ($N_e = N/2$), for magnetic fluxes $-1/2 < \phi/\phi_0 < 1/2$. In the half-filled band case, the uncorrelated part of the disorder reduces the persistent current while the correlated part enhances it, in such a way that for $\alpha^2 < \varepsilon_0^2/2$ the current decreases with the disorder, while for $\alpha^2 > \varepsilon_0^2/2$ it increases with it. Also, while showing a specific dependence on the flux, the disorder effect has the same dependence on the parity of $N_e$ as the pure system-free electron current. In contrast, at low filling of the energy band, the disorder-induced effect in the persistent current depends critically on the parity: due to a peculiar dependence on the flux, it yields a reduction of the current for odd $N_e$ and an enhancement of it for even $N_e$. The observability of the effects of weak correlated disorder on persistent current in the half-filled band case is restricted to ring sizes in the nanoscale range, for which no measurements presently exist.

## 1. Introduction

The study of persistent current in small metallic rings threaded by a magnetic flux has a long history, starting with the basic papers of London [1] and Hund [2]. It has been boosted in recent years with the appearance of the seminal paper of Büttiker, Imry and Landauer [3] for one-dimensional rings. Important aspects related to the effects of disorder and of electron–electron interaction on the persistent current have been reviewed and compared with experimental observations [4–6] in well-known monographs [7, 8]and in review articles [9]. An important unsolved problem remains, however, to reconcile theoretical and experimental results for the persistent current, particularly in the case where the current averaged over many experimental realizations of isolated disordered rings of a given metal has been measured [4]. In this case the theoretical results for the ensemble-averaged current are between one or two orders of magnitude lower [7] than the experimental values [4], depending on whether electron–electron interaction effects are included or not. However, the electron interaction effects are not easy to calculate and no definitive answer as to their precise role seems to exist since there are even models in which Coulomb interactions act to reduce the persistent current rather than to enhance it [10].

In the present paper we examine another effect which may substantially enhance the persistent current in a disordered ring subjected to a magnetic flux. This effect exists when the disordered potential is not perfectly random as a result of short-range correlations. More precisely, we consider an Anderson tight-binding model of a ring with an even number $N = 2M$ of one level atomic sites (of spacing $a = 1$) whose energies $\varepsilon_n$ fluctuate randomly about a fixed free atom level

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chosen as the zero of energy. As usual the $N$ site energies are assumed to be identically distributed independent random variables. In order to account for short-range correlations we extend the model as follows: we divide the ring up into pairs of nearest-neighbour atomic sites (dimers), namely the pairs (1, 2), (3, 4) ... $(2M-1, 2M)$, where the sites within individual pairs are assumed to be Gaussian correlated, whereas sites belonging to different pairs are uncorrelated. Including the usual autocorrelation, the Gaussian correlation of site energies is then described by the averages

$$\langle \varepsilon_n \rangle = 0,$$
$$\langle \varepsilon_m \varepsilon_n \rangle = \varepsilon_0^2 \delta_{\min} + \alpha^2 \left(\delta_{m,2p-1}\delta_{n,2p} + \delta_{m,2p}\delta_{n,2p-1}\right). \quad (1)$$

The intersite coupling term in (1) describes short-range structural (dimer) correlations of an otherwise uncorrelated (white-noise) random potential. In the following we refer to the Gaussian model (1) as an Anderson random dimer model (ARDM) which was first discussed in the context of localization on a linear chain [11], in the case $\alpha^2 = \varepsilon_0^2$. It differs from the random dimer model (RDM) introduced earlier by Phillips and coworkers [12, 13] for demonstrating the existence of delocalized states in a one-dimensional system with correlated disorder. This model considers chains of $N$ lattice sites composed of clusters of host atoms $a$ of site energy $\varepsilon_a$ separated by clusters of defect atoms of energy $\varepsilon_b$ occurring randomly but in pairs of nearest neighbours [12, 13]. Apart from its binary character this system differs from our ARDM in that clusters of $a$ atoms are not restricted to even numbers of atoms unlike the clusters composed of $b$ atoms. The RDM model of Phillips *et al* leads to the existence of $\sqrt{N}$ delocalized states in the linear chain lattice [12, 13]. In contrast, the ARDM model (for $\alpha^2 = \varepsilon_0^2$) on a linear chain lattice leads to localized states only, with a localization length $\xi$ given by [11]

$$\frac{1}{\xi} \simeq \frac{\varepsilon_0^2 E^2}{4(4-E^2)} = \frac{E^2}{2\xi_0}, \quad (2)$$

for weak disorder. Here $E = 2\cos k$ is the energy band (in units of a constant nearest-neighbour hopping parameter $V$) of states of wavenumber $k$ of the ordered lattice and $\xi_0$ is the weak disorder Thouless localization length for uncorrelated Gaussian disorder in one dimension. The expression (2) is valid at energies $E$ except for some special values within the energy band (including $E = 0$) where the weak disorder treatment must be corrected for Kappus–Wegner-type anomalies [11, 14]. It follows from (2) that the localization length near the band centre is strongly increased with respect to $\xi_0$ by the effect of disorder correlation.

For the tight-binding system on a ring threaded by a magnetic flux in the direction perpendicular to the ring the Schrödinger equation reduces to the set of difference equations [15, 16]

$$-e^{i\frac{2\pi}{N}\frac{\phi}{\phi_0}}\varphi_{n+1} - e^{-i\frac{2\pi}{N}\frac{\phi}{\phi_0}}\varphi_{n-1} + \varepsilon_n\varphi_n = E\varphi_n, \quad n = 2, 3, \ldots, N-1, \quad (3)$$

$$-e^{i\frac{2\pi}{N}\frac{\phi}{\phi_0}}\varphi_2 - e^{-i\frac{2\pi}{N}\frac{\phi}{\phi_0}}\varphi_N + \varepsilon_1\varphi_1 = E\varphi_1, \quad (4)$$

$$-e^{i\frac{2\pi}{N}\frac{\phi}{\phi_0}}\varphi_1 - e^{-i\frac{2\pi}{N}\frac{\phi}{\phi_0}}\varphi_{N-1} + \varepsilon_N\varphi_N = E\varphi_N, \quad (5)$$

which embody the familiar flux-modified (twisted) boundary condition [3, 16] describing the effect of the magnetic flux. Here $\phi_0 = hc/e$ is the flux quantum (with $h$ the Planck constant, $c$ the velocity of light and $-e$ the electron charge), $\varphi_n$ is the amplitude of an eigenstate wavefunction at site $n$, $E$ and $\varepsilon_n$, are the corresponding eigenvalue and site energies in units of minus a constant nearest-neighbour hopping parameter. The equilibrium persistent current carried by the $k$th one-electron eigenstate of (3)–(5) is

$$I_k = -c\frac{\partial E_k}{\partial \phi}, \quad (6)$$

and the total persistent current in a ring containing $0 < N_e \leqslant N$ spinless electrons in the zero-temperature ground state is given by

$$I = \sum_k I_k, \quad (7)$$

where the summation extends over the $N_e$ lowest one-electron eigenstates of (3)–(5).

Persistent current has been studied recently in the RDM of Dunlap *et al* [12] in several papers [17–20]. In particular, Liu *et al* [17] have shown that in the model of Dunlap *et al* the persistent current is enhanced by the disorder correlation to values approaching the current in an ordered system if the Fermi level coincides with the energy of a delocalized state. On the other hand, their numerical calculations indicate that the persistent current is strongly suppressed when no delocalized state is present near the Fermi level [17].

The study of the persistent current in the ARDM is of interest in view of its specific localization properties discussed above. In particular, this study may allow us to clarify whether the presence of a correlation-induced delocalized state at the Fermi level is indispensable for obtaining large persistent currents as discussed by the authors of [17] and [18] for the RDM. These are our main motivations for the present work. The ensemble-averaged energy eigenvalues for the ARDM model for weak disorder are discussed in section 2, using the general perturbation expressions for the eigenvalues of equations (3)–(5) derived in [16]. The detailed study of the ensemble-averaged persistent current successively for a system of $N_e \ll N$ spinless electrons occupying a small portion of the energy band of the ring described by (3)–(5), and for a system of $N_e = N/2$ electrons occupying the lower half of the energy band at zero temperature, is presented and discussed in section 3. Some final remarks are given in section 4.

## 2. The perturbed energy levels of the ring

Exact general expressions for the one-electron energy levels of the ring threaded by a magnetic flux and perturbed by a weak site energy disorder have been derived from (3)–(5) in [16], using an exact transfer matrix formalism and expanding the transfer matrix to second order in the disorder. In the absence of disorder the energy levels are given by the familiar tight-binding results [15, 16]:

$$E_k^0(\phi) = E_k^0 = -2\cos\frac{2\pi}{N}\left(k + \frac{\phi}{\phi_0}\right), \quad (8)$$

where $k = 0, \pm 1, \pm 2, \ldots$, and the solution of the eigenvalue equation yields the following exact expressions for the first- and second-order perturbations of the energy levels [16]:

$$E_k = E_k^0 + E_k^{(1)} + E_k^{(2)} + \cdots \tag{9}$$

$$E_k^{(1)} \equiv E^{(1)} = \frac{1}{N}\sum_{n=1}^{N} \varepsilon_n, \tag{10}$$

$$E_k^{(2)} = \frac{1}{N \sin q_k \sin N q_k} \sum_{n=2}^{N}\sum_{m=1}^{n-1} (E^{(1)} - \varepsilon_m)(E^{(1)} - \varepsilon_n) \times \sin(n-m)q_k \sin(N-n+m)q_k, \tag{11}$$

where

$$q_k = \frac{2\pi}{N}\left(k + \frac{\phi}{\phi_0}\right). \tag{12}$$

As recalled in [16] the weak disorder expansion breaks down at flux values equal to half-integer multiples of $\phi_0$ including $\phi = 0$ where (11) diverges[1]. Such divergences are familiar in other perturbative studies of persistent current [22] and are due to the degeneracies of the unperturbed electron energies (8) at these flux values.

As in our earlier work [16] we are interested in the change of persistent current induced by the energy correction (11) averaged over the disorder. The derivation of the closed form of (11) averaged over the correlated disorder defined by (1) involves the following steps:

(1) for each one of the four disorder factors $(E^{(1)})^2$, $-\varepsilon_m E^{(1)}$, $E^{(1)}\varepsilon_n$ and $\varepsilon_m\varepsilon_n$ (with $E^{(1)}$ defined by (10)) which enter in the site summations in (11), we identify explicitly the individual nearest-neighbour pair terms with a non-vanishing correlation (1), in addition to the autocorrelation terms.

(2) After performing the disorder averaging, using (1), the various contributions reduce to combinations of geometric series over sites, which are then summed in closed form. As a guide to our calculations we list in the appendix the final explicit results obtained for the four distinct disorder terms in (11). The sum of the contributions (A.2)–(A.5) leads, after further reduction, to the following exact expression for the averaged disorder effect in the ARDM:

$$\langle E_k^{(2)}\rangle = \langle E_k^{(2)}\rangle^{\mathrm{uncorr}} + \langle E_k^{(2)}\rangle^{\mathrm{corr}}, \tag{13}$$

where

$$\langle E_k^{(2)}\rangle^{\mathrm{uncorr}} = \frac{\varepsilon_0^2}{4\sin q_k}\left[\left(1+\frac{1}{N}\right)\cot\frac{2\pi\phi}{\phi_0} - \frac{1}{N}\cot q_k\right], \tag{14}$$

and

$$\begin{aligned}\langle E_k^{(2)}\rangle^{\mathrm{corr}} = \frac{\alpha^2}{4}\Bigg\{ & 2\left(\cos q_k - \cot\frac{2\pi\phi}{\phi_0}\sin q_k\right) - \frac{3}{N}\frac{\cot(2\pi\phi/\phi_0)}{\sin q_k} - \frac{1}{N^2 \sin\frac{2\pi\phi}{\phi_0}\sin q_k} \\ & \times\Bigg[\frac{e^{-i\frac{2\pi\phi}{\phi_0}}}{1-e^{-2iq_k}}\Bigg(\frac{i\left(1-e^{i\frac{4\pi\phi}{\phi_0}}\right)}{\sin 2q_k} + \frac{1}{1-e^{2iq_k}} \\ & \times\left(1+e^{2iq_k} - e^{\frac{i4\pi\phi}{\phi_0}}\right) - \frac{1}{1-e^{4iq_k}}e^{i\frac{4\pi\phi}{\phi_0}}(1+e^{6iq_k}) \\ & - 3\frac{N}{2} - 1 - (N-1)e^{4iq_k} - \frac{N}{2}e^{-4iq_k}\Bigg) + \mathrm{c.c.}\Bigg]\Bigg\}.\end{aligned} \tag{15}$$

Here $\langle E_k^{(2)}\rangle^{\mathrm{uncorr}}$ represents the averaged energy correction resulting from the random potential in the absence of correlation, which has been studied earlier [16], and $\langle E_k^{(2)}\rangle^{\mathrm{corr}}$ represents the effect of the correlation of the disorder described by the dimer model of [11]. Equations (9) and (13)–(15) are used in the following section for studying the ensemble-averaged persistent currents.

## 3. The persistent current in the ring

We first recall the results for the persistent current in the pure (non-disordered) tight-binding ring obtained from equations (6)–(8). The energy levels (8) occupied by the $N_e$ spinless electrons differ for odd and for even $N_e$, as well as for different domains of relative magnetic flux $\phi/\phi_0$, as is well known [15]. The sets of occupied $k$ levels entering in the calculation of the total current in various cases may be inferred from the set of intersecting parabolas representing the energy level spectrum as a function of flux in the free-electron limit (see, e.g., figure 2 in [15]). They are defined by the values $k = 0, \pm 1, \pm 2, \ldots, \pm(N_e - 1)/2$ for odd $N_e$ and $-1/2 < \phi/\phi_0 < 1/2$; and by $k = 0, \pm 1, \ldots, \pm(N_e/2 - 1), -N_e/2$ for $0 < \phi/\phi_0 < 1/2$ and by $k = 0, \pm 1, \ldots, \pm(N_e/2 - 1), N_e/2$ for $-1/2 < \phi/\phi_0 < 0$ for even $N_e$, respectively. The summation of the contributions of the various levels (8) reduces to geometric progressions, leading to the following mostly well-known results for pure system currents $I^{(0)}$ [15, 17]:

$$I^{(0)} = -I_0\frac{\sin(2\pi\phi/N\phi_0)}{\sin\pi/N} \simeq -I_0\frac{2\phi}{\phi_0}, \quad \left(\text{odd } N_e,\ -\tfrac{1}{2} < \phi/\phi_0 < \tfrac{1}{2}\right), \tag{16}$$

$$I^{(0)} = -I_0\frac{\sin(\pi/N)(2\phi/\phi_0 - 1)}{\sin\pi/N} \simeq -I_0\left(\frac{2\phi}{\phi_0} - 1\right), \quad \left(\text{even } N_e,\ 0 < \phi/\phi_0 < \tfrac{1}{2}\right), \tag{17a}$$

$$I^{(0)} = -I_0\frac{\sin(\pi/N)(2\phi/\phi_0 + 1)}{\sin\pi/N} \simeq -I_0\left(\frac{2\phi}{\phi_0} + 1\right), \quad \left(\text{even } N_e,\ -\tfrac{1}{2} < \phi/\phi_0 < 0\right), \tag{17b}$$

$$I_0 = \frac{e v_F}{N}, \qquad v_F = \frac{4\pi}{h}\sin k_F, \qquad k_F = \frac{\pi N_e}{N}, \tag{18}$$

where the approximate limiting forms correspond to the limit $N \to \infty$ and coincide in the case of (16) and (17a) with

[1] General expressions for energy levels perturbed by a weak disorder similar to (8)–(12) have been derived earlier in the case of a ring threaded by a non-Hermitian field in [21]. The interest in this problem of non-Hermitian quantum mechanics arose from the study of the pinning of vortices by columnar defects in a superconductor.

earlier analytical results for free electrons [15]. $v_F$ and $k_F$ in (18) denote the tight-binding Fermi velocity and the Fermi momentum, respectively [16]. The limiting free-electron expressions in (16), (17*a*) and (17*b*) exhibit the familiar sawtoothed currents shown in figures (3a) and (3b) of [15] (whose legends must be interchanged!).

We now study the effect of the correlated disorder on the persistent current obtained from (6)–(10) and (13)–(15) for a system of $N_e$ spinless electrons in the $T = 0$ ground state. Our general discussion is made systematic by considering successively the case of low filling, $N_e \ll N$, of the energy band and the case of higher filling exemplified by the half-filled band case, $N_e = N/2$.

### *3.1. Low filling of energy band*

For occupied levels with quantum numbers $k \ll N$ and magnetic flux restricted by (16), (17*a*) and (17*b*) we use

$$\sin q_k \simeq q_k = \frac{2\pi}{N}\left(k + \frac{\phi}{\phi_0}\right), \tag{19}$$

and by expanding (14) and (15) to lowest order for large $N$ we obtain

$$\langle E_k^{(2)}\rangle = \frac{\varepsilon_0^2}{4q_k}\left(\cot\frac{2\pi\phi}{\phi_0} - \frac{1}{Nq_k}\right) - \frac{3\alpha^2}{4Nq_k^2} + \mathrm{O}[(q_k)^0 = 1], \tag{20}$$

where

$$\langle E_k^{(2)}\rangle^{\text{uncorr}} = \frac{\varepsilon_0^2}{4q_k}\left(\cot\frac{2\pi\phi}{\phi_0} - \frac{1}{Nq_k}\right), \tag{21}$$

is the uncorrelated disorder perturbation at low band filling obtained from (14). Equation (20) will allow us to discuss the current generated by a system of $N_e \ll N$ electrons.

*3.1.1. Single-electron current.* It is instructive to briefly discuss the effect of correlated and uncorrelated disorder on the persistent current for a single electron on the lowest level ($k = 0$) of the energy band (8) for $-1/2 < \phi/\phi_0 < 1/2$. From (20) and (6) we obtain

$$\langle I_{k=0}\rangle_{\text{disorder}} = I_0\left(\frac{N}{4\pi}\right)^2\frac{\phi_0}{\phi}\left[\frac{\varepsilon_0^2}{\sin^2(2\pi\phi/\phi_0)} + \frac{\varepsilon_0^2\phi_0}{2\pi\phi}\cot\frac{2\pi\phi}{\phi_0} - 2(\varepsilon_0^2 + 3\alpha^2)\left(\frac{\phi_0}{2\pi\phi}\right)^2\right], \tag{22}$$

where $I_0 = (4\pi^2 e)/Nh$. It follows from (22) that the correlated disorder generally leads to an enhancement of persistent current with respect to the pure system result, $I_{k=0} = -I_0 2\phi/N\phi_0$, obtained from (8). In contrast the corresponding expression for the current induced by uncorrelated disorder vanishes for $\phi/\phi_0 \to 0$ and leads to suppression of persistent current at larger flux within the range (16).

*3.1.2. Low band filling.* At low band filling the occupied energy levels in the ring below the Fermi level correspond to small $q_k$ values (for large $N$), so that the terms involving $\sin q_k$ and related small quantities in the denominators dominate in the disorder perturbation (14) and (15). By expanding the denominators in question to leading order in $q_k$ and collecting terms we obtained the expression (20) for $\langle E_k^{(2)}\rangle$ which we now use for calculating the persistent current induced by the system of $N_e$ electrons in the ground state when $1 \ll N_e \ll N$. The averaged persistent current from the $k$th level is given by

$$\langle I_k\rangle_{\text{disorder}} = \frac{\pi e}{2h}\frac{1}{Nq_k}\left[\frac{\varepsilon_0^2 N}{\sin^2(2\pi\phi/\phi_0)} + \frac{\varepsilon_0^2}{q_k}\cot\frac{2\pi\phi}{\phi_0} - \frac{2(\varepsilon_0^2 + 3\alpha^2)}{Nq_k^2}\right]. \tag{23}$$

A simple analytic procedure for performing the summation of the currents (23) from the $N_e$ lowest levels of the energy band (9) is to replace the summation by an integration. For this purpose we use the series summation formula of Euler–Maclaurin [23]:

$$\sum_{k=k_-}^{k_+} f_k = \int_{K_-}^{K_+} f(k)\,\mathrm{d}k - \tfrac{1}{2}[f(K_-) + f(K_+)],$$
$$K_- = k_- - 1, \qquad K_+ = k_+ + 1, \tag{24}$$

where we have retained only the leading boundary term of the general formula [23]. Here $k_-$ and $k_+$ denote, respectively, the smallest and the largest value of the quantum number $k$ labelling the occupied levels in the energy band of the ring. From the spectra of occupied energy levels detailed above for the domains $-1/2 < \phi/\phi_0 < 1/2$ for odd and for even $N_e$ we have $k_+ = -k_- = (N_e - 1)/2$ for odd $N_e$; $k_+ = N_e/2 - 1$ and $k_- = -N_e/2$ for even $N_e$ with $\phi > 0$; and $k_+ = N_e/2$, $k_- = -N_e/2 + 1$ for even $N_e$ and $\phi < 0$. We thus obtain the following values for $q_k$ at the lower and upper limits of the integral in (24):

$$q_{K_-} = \frac{\pi}{N}\left(-N_e - 1 + \frac{2\phi}{\phi_0}\right),$$
$$q_{K_+} = \frac{\pi}{N}\left(N_e + 1 + \frac{2\phi}{\phi_0}\right), \tag{25}$$
$$\left(\text{odd } N_e, -\frac{1}{2} < \frac{\phi}{\phi_0} < \frac{1}{2}\right),$$

$$q_{K_-} = \frac{\pi}{N}\left(-N_e + \frac{2\phi}{\phi_0}\right),$$
$$q_{K_+} = \frac{\pi}{N}\left(N_e + 2 + \frac{2\phi}{\phi_0}\right), \tag{26a}$$
$$\left(\text{even } N_e, -\frac{1}{2} < \frac{\phi}{\phi_0} < 0\right)$$

$$q_{K_-} = \frac{\pi}{N}\left(-N_e - 2 + \frac{2\phi}{\phi_0}\right),$$
$$q_{K_+} = \frac{\pi}{N}\left(N_e + \frac{2\phi}{\phi_0}\right), \tag{26b}$$
$$\left(\text{even } N_e, 0 < \frac{\phi}{\phi_0} < \frac{1}{2}\right).$$

which are valid for arbitrary $0 < N_e < N$. Having discussed the case $N_e = 1$ in section 3.1.1 above we now focus mainly on values $N_e \gg 1$ for which

$$q_{K_+} \simeq -q_{K_-} = \frac{\pi N_e}{N}\left(1 + \mathrm{O}\left(\frac{1}{N_e}\right)\right), \qquad N_e \gg 1, \quad (27)$$

in the various cases detailed in (25) and (26). This will be sufficient indeed for illustrating the qualitative differences between these cases.

The total persistent current (7) obtained from (23) involves three types of sums over occupied levels, namely $S_1 = \sum_k q_k^{-1}$, $S_2 = \sum_k q_k^{-2}$ and $S_3 = \sum_k q_k^{-3}$. We recall the occupied levels in the various domains of flux, namely $k = -(N_e - 1)/2, -(N_e - 1)/2 + 1, \ldots, 0, 1, \ldots (N_e - 1)/2$ for odd $N_e$ and $-1/2 < \phi/\phi_0 < 1/2$, $k = -N_e/2 + 1, -N_e/2 + 2, \ldots, 0, \ldots N_e/2 - 1, N_e/2$ for even $N_e$ and $-1/2 < \phi/\phi_0 < 0$, and finally, $k = -N_e/2, -N_e/2 + 1, \ldots, 0, \ldots N_e/2 - 1$, for even $N_e$ and $0 < \phi < 1/2$. The series $S_1$ which does not converge for $k \to \infty$ requires special care. Using (12), we rewrite it in the following forms:

$$S_1 = \frac{N\phi_0}{2\pi\phi}(1-2J), \qquad \text{for odd } N_e, \; -\frac{1}{2} < \frac{\phi}{\phi_0} < \frac{1}{2}, \quad (28)$$

$$S_1 = \frac{N\phi_0}{2\pi\phi}(1-2J) + \frac{1}{q_{k_+}}, \quad \text{for even } N_e, \; -\frac{1}{2} < \frac{\phi}{\phi_0} < 0, \quad (29a)$$

$$S_1 = \frac{N\phi_0}{2\pi\phi}(1-2J) + \frac{1}{q_{k_-}}, \quad \text{for even } N_e, \; 0 < \frac{\phi}{\phi_0} < \frac{1}{2}, \quad (29b)$$

$$J = \sum_{k=1}^{p} \frac{1}{k^2 - (\phi/\phi_0)^2}, \quad (30)$$

with $p = k_+$ in the case of (28), $p = k_+ - 1$ in the case of (29a) and $p = k_+$ in the case of (29b).

In applying (24) for performing the summation over the occupied levels in (30) we encounter a difficulty which is the fact that the integral is not defined since its lower limit (zero) leads to an imaginary term. This difficulty may be resolved by introducing a small $k$ cutoff for the domain of integration, say at $k \equiv k_c = 1$. This is justified since the lowest discrete levels contributing to the integral are the levels $k = \pm 1$, the effect of the level $k = 0$ having been separated out in the first term on the right-hand side of (28), (29a) and (29b). With this regularization we obtain

$$J = \frac{\phi_0}{2\phi}\left[\ln\left(\frac{1-\phi/\phi_0}{1+\phi/\phi_0}\right) + \frac{4\phi}{N_e\phi_0}\right] - \frac{\phi_0^2}{2(\phi_0^2 - \phi^2)} + \mathrm{O}\left(\frac{1}{N_e^2}\right). \quad (31)$$

On the other hand, by summing $S_2$ and $S_3$ using (24), we obtain

$$S_2 = -\frac{N}{2\pi}\left(\frac{1}{q_{K_+}} - \frac{1}{q_{K_-}}\right) - \frac{1}{2}\left(\frac{1}{q_{K_+}^2} + \frac{1}{q_{K_-}^2}\right), \quad (32)$$

$$S_3 = -\frac{N}{4\pi}\left(\frac{1}{q_{K_+}^2} - \frac{1}{q_{K_-}^2}\right) - \frac{1}{2}\left(\frac{1}{q_{K_+}^3} + \frac{1}{q_{K_-}^3}\right), \quad (33)$$

and using the definition (25) and (26a), (26b) the leading explicit forms of (28), (29a), (29b) and (32) and (33) are given by

$$S_1 = \frac{N\phi_0}{2\pi\phi}(1-2J), \qquad \text{odd } N_e, \quad (34)$$

$$S_1 = \frac{N\phi_0}{2\pi\phi}(1-2J) + \frac{N}{\pi N_e}\left[1 + \mathrm{O}\left(\frac{1}{N_e}\right)\right], \quad \text{even } N_e, \; -\frac{1}{2} < \frac{\phi}{\phi_0} < 0, \quad (35a)$$

$$S_1 = \frac{N\phi_0}{2\pi\phi}(1-2J) - \frac{N}{\pi N_e}\left[1 + \mathrm{O}\left(\frac{1}{N_e}\right)\right], \quad \text{even } N_e, \; 0 < \frac{\phi}{\phi_0} < \frac{1}{2}, \quad (35b)$$

$$S_2 = -\frac{N^2}{\pi^2 N_e}\left[1 + \mathrm{O}\left(\frac{1}{N_e}\right)\right], \quad (36)$$

$$S_3 = \frac{2\phi}{\phi_0}\left(\frac{N}{\pi N_e}\right)^3\left[1 + \mathrm{O}\left(\frac{1}{N_e}\right)\right], \quad (37)$$

where the limiting forms (36) and (37) are valid for even as well as for odd $N_e$, in the domain $-1/2 < \phi/\phi_0 < 1/2$.

Finally, using (23) and (34)–(37), the change in the persistent current (7) due to the disorder is given by

$$\langle I\rangle_{\text{disorder}} = \frac{I_0 N^3 \varepsilon_0^2}{8\pi N_e}\left\{\left[\frac{\phi_0}{2\pi\phi}(1-2J) + Q\right] \times \frac{1}{\sin^2(2\pi\phi/\phi_0)} - \frac{1}{\pi^2 N_e}\cot\frac{2\pi\phi}{\phi_0} + \mathrm{O}\left(\frac{1}{N_e^2}\right)\right\}, \quad (38)$$

where $Q = 0$ for odd $N_e$, $Q = (\pi N_e)^{-1}$ for even $N_e$ with $-1/2 < \phi/\phi_0 < 0$ and $Q = -(\pi N_e)^{-1}$ for even $N_e$ with $0 < \phi/\phi_0 < 1/2$.

It follows from (38) that, for $1 \ll N_e \ll N$, the effect of the disorder is dominated by the form of $J$ in (31), which is negative for both signs of the magnetic flux $\phi$. This shows that for odd $N_e$ the disorder reduces the persistent current with respect to the pure system result (16) while enhancing it with respect to the corresponding pure system values (17a) and (17b) for even $N_e$.

We conclude that, while the correlation effect may efficiently offset the effect of an uncorrelated potential on the persistent current both in the case of a single electron (see section 3.1.1) and in that of a gas of a large number of electrons (see the case $N_e = N/2$ in section 3.2 below), it does not affect the effect of uncorrelated disorder on the persistent current in systems with $1 \ll N_e \ll N$ at low order.

### 3.2. *Half-filled band*

In the case of a half-filled band the terms proportional to $1/N$ and to $1/N^2$ in the energy level perturbations (14) and (15) may be ignored relative to the remaining terms of order one for energy levels (8) near the Fermi level. In this case we thus have from (14) and (15)

$$\langle E_k^{(2)}\rangle^{\text{uncorr}} \simeq \frac{\varepsilon_0^2}{4\sin q_k}\cot\frac{2\pi\phi}{\phi_0}, \quad (39)$$

$$\langle E_k^{(2)}\rangle^{\rm corr} \simeq \frac{\alpha^2}{2}\left(\cos q_k - \cot\frac{2\pi\phi}{\phi_0}\sin q_k\right). \tag{40}$$

The persistent current due to the effect of the uncorrelated random potential (39) has been discussed in [16] for a half-filled band for odd $N_e$ in the range $-1/2 < \phi/\phi_0 < 1/2$ and for even $N_e$ in the range $0 < \phi/\phi_0 < 1$, using the Euler–Maclaurin series summation formula. However, throughout the present work we consider the typical domain $-1/2 < \phi/\phi_0 < 1/2$ for the detailed analyses of the effects of correlated disorder in the persistent current. This seems more useful since recent first numerical results for persistent currents in disordered rings with a correlated random potential have been presented for the range $-1/2 < \phi/\phi_0 < 1/2$ only [17–19]. From (39) the effect of the uncorrelated random potential on the persistent current in the $k$th level is given by

$$\langle I_k\rangle_{\rm uncorr} = \frac{\pi e}{2h}\frac{\varepsilon_0^2}{\sin^2(2\pi\phi/\phi_0)}\frac{1}{\sin q_k} + {\rm O}(1/N). \tag{41}$$

whose summation for the $N_e$ lowest occupied levels of the energy band (8) in the domains $-1/2 < \phi/\phi_0 < 0$ and $0 < \phi/\phi_0 < 1/2$, respectively, is performed using the Euler–Maclaurin formula (24). Using (18), this yields the following final result for the effect of the uncorrelated disorder on the mean persistent current in the half-filled band:

$$\langle I\rangle_{\rm uncorr} = I_0\frac{N\varepsilon_0^2}{8\sin^2(2\pi\phi/\phi_0)} \times\left[-\frac{N}{4\pi}\ln\frac{(1+\cos q_{K_+})(1-\cos q_{K_-})}{(1-\cos q_{K_+})(1+\cos q_{K_-})} -\frac{1}{2}\left(\frac{1}{\sin q_{K_-}}+\frac{1}{\sin q_{K_+}}\right)\right], \tag{42}$$

in terms of the $q_k$ values (25), (26$a$) and (26$b$) for $N_e = N/2$, near the upper and lower boundary values $k_+$ and $k_-$ of the domain of occupied $k$ levels and for flux values within the interval $(-\phi_0/2, \phi_0/2)$. Equation (42) may be readily simplified for $N_e = N/2 \gg 1$ by expanding the square bracket to leading order in $1/N$, using (25), (26$a$) and (26$b$). This yields

$$\langle I\rangle_{\rm uncorr} = I_0\frac{N\varepsilon_0^2}{8\sin^2(2\pi\phi/\phi_0)}A, \tag{43}$$

$$A = \frac{2\phi}{\phi_0} + {\rm O}(1/N^2), \qquad \text{odd } N_e,\ -\frac{1}{2} < \frac{\phi}{\phi_0} < \frac{1}{2}, \tag{44}$$

$$A = 1 + \frac{2\phi}{\phi_0} + {\rm O}(1/N^2), \qquad \text{even } N_e,\ -\frac{1}{2} < \frac{\phi}{\phi_0} < 0, \tag{45a}$$

$$A = -1 + \frac{2\phi}{\phi_0} + {\rm O}(1/N^2), \qquad \text{even } N_e,\ 0 < \frac{\phi}{\phi_0} < \frac{1}{2}, \tag{45b}$$

where (43) with $A$ defined by (44) or (45$b$) has been obtained earlier in [16].

The persistent current due to the correlation for an electron on the $k$th level is, from (6) and (40),

$$\langle I_k\rangle_{\rm corr} = -\frac{\pi e}{h}\frac{\alpha^2}{\sin^2(2\pi\phi/\phi_0)}\sin q_k + {\rm O}(1/N), \tag{46}$$

which leads to the following exact results for the persistent current for the system of $N_e$ spinless electrons occupying the lower half of the energy band of the system:

$$\langle I\rangle_{\rm corr} = -I_0\frac{N\alpha^2}{4\sin^2(2\pi\phi/\phi_0)}\frac{\sin(2\pi\phi/N\phi_0)}{\sin\pi/N} \simeq -I_0\left(\frac{2\phi}{\phi_0}\right)\frac{N\alpha^2}{4\sin^2(2\pi\phi/\phi_0)}, \quad (\text{odd } N_e,\ -1/2 < \phi/\phi_0 < 1/2), \tag{47}$$

$$\langle I\rangle_{\rm corr} = -I_0\frac{N\alpha^2}{4\sin^2(2\pi\phi/\phi_0)}\frac{\sin\frac{\pi}{N}\left(\frac{2\phi}{\phi_0}\pm 1\right)}{\sin\pi/N} \simeq -I_0\left(\frac{2\phi}{\phi_0}\pm 1\right)\frac{N\alpha^2}{4\sin^2(2\pi\phi/\phi_0)}, \quad (\text{even } N_e,\ +\text{ sign for } -1/2 < \phi/\phi_0 < 0,\ -\text{ sign for } 0 < \phi/\phi_0 < 1/2), \tag{48}$$

By comparing these expressions with the pure system currents (16), (17$a$) and (17$b$) it follows that the effect of the correlation of the random potential is, in all cases, to enhance the persistent current.

Finally the total average persistent current $\langle I\rangle$ in the ring is given by the sum of free-electron currents (large $N$ limits of pure tight-binding system currents, equations (16), (17$a$) and (17$b$)) and the changes in the persistent current induced by the disorder via the correlations of the random potential (equations (47) and (48)) and via the random potential in the absence of correlation (equations (43) and (45)):

$$\langle I\rangle = -I_0\left(\frac{2\phi}{\phi_0}\right)\left[1 - \frac{N(\varepsilon_0^2 - 2\alpha^2)}{8\sin^2(2\pi\phi/\phi_0)}\right], \quad \text{odd } N_e,\ -\frac{1}{2} < \frac{\phi}{\phi_0} < \frac{1}{2}, \tag{49}$$

$$\langle I\rangle = -I_0\left(\frac{2\phi}{\phi_0}+1\right)\left(1 - \frac{N(\varepsilon_0^2 - 2\alpha^2)}{8\sin^2(2\pi\phi/\phi_0)}\right), \quad \text{even } N_e,\ -\frac{1}{2} < \frac{\phi}{\phi_0} < 0, \tag{50a}$$

$$\langle I\rangle = -I_0\left(\frac{2\phi}{\phi_0}-1\right)\left(1 - \frac{N(\varepsilon_0^2 - 2\alpha^2)}{8\sin^2(2\pi\phi/\phi_0)}\right), \quad \text{even } N_e,\ 0 < \frac{\phi}{\phi_0} < \frac{1}{2}, \tag{50b}$$

with $I_0$ defined in (18). These expressions are invalid near $\phi = 0$, which is a consequence of the breakdown of the perturbation expression (11) for flux values equal to half-integer multiples of the flux quantum, as mentioned earlier.

The expressions (49), (50$a$) and (50$b$) indicate that the disorder acts to renormalize the free-particle persistent currents (16), (17$a$) and (17$b$) by a common factor. In particular, it follows that the correlation of the random potential leads to a systematic increase of the persistent current proportional to $\alpha^2$. However, the important feature of (50$a$) and (50$b$) is that, for $\alpha^2$ less than the critical value $\alpha^2 \equiv \alpha_c^2 = \varepsilon_0^2/2$, the persistent current is reduced by the correlated disorder while for $\alpha^2 > \alpha_c^2$ it is enhanced by it for any parity. In this respect, the results for the persistent current at low band filling, $1 \ll N_e \ll N$, discussed in section 3.1 above show an interesting asymmetry. Indeed, in this case the effect of the correlated disorder is to reduce the persistent current for odd $N_e$ and to enhance it for even $N_e$. This is a consequence of the fact that the flux dependence of the persistent current (38) induced by the disorder does not follow the simple linear scalings of the pure system currents (16), (17*a*) and (17*b*).

### *3.3. Discussion of the results*

In this subsection we discuss the restrictions on ring lengths $N$ and on relative flux values in (49), (50*a*) and (50*b*) which are imposed by our non-degenerate perturbation study of the effect of the disorder on the energy levels of the ring in the presence of the applied flux. We focus mainly on the case of the half-filled energy band where the effects of the disorder on the persistent current may be observed for a wide range of nanoscale ring parameters, as shown below.

First, the perturbation expansion (9) in terms of the random site energies relative to the fixed intersite hopping parameter implies, by definition,

$$|\varepsilon_0| \ll 1, |\alpha| \ll 1, \tag{51}$$

which reflects the fact that the first-order correction to the energy levels, $E_k^{(0)}$, of the pure system is small. Next, the typical value of the first-order shift of energy levels due to the disorder, $\sqrt{\langle E_k^{(1)2}\rangle} = \sqrt{(\varepsilon_0^2+\alpha^2)/N}$, must be small compared to the spacing, $|\Delta|$, of the energy levels of the pure system. From (8) we obtain

$$\Delta = E_{k+1}^{(0)}(\phi) - E_k^{(0)}(\phi) = \frac{4\pi}{N}\sin\frac{2\pi}{N}\left(k+\frac{1}{2}+\frac{\phi}{\phi_0}\right),$$

which leads to the condition

$$\sqrt{N}\sqrt{\varepsilon_0^2+\alpha^2} \ll 4\pi \sin\frac{2\pi}{N}\left(\frac{1}{2}+\frac{\phi}{\phi_0}\right) \simeq 4\pi, \tag{52}$$

at the Fermi level (where $k = \pm N_e/2$) in the half-filled band case. This condition which is important for close-spaced level systems (large $N$) expresses that disorder acts as a small perturbation on the (observable) excitation frequencies defined by $\Delta$. Since, for band fillings $N_e \ll N$, equation (52) restricts the discussion to rings of perimeters less than a few nanometres, we focus, in the remainder of this subsection, on the half-filled band case $N_e = N/2$, where our analysis covers a much wider range of nanometric ring sizes. Also, since here we are mainly interested in analysing the effect of small random potential correlations ($\alpha^2 \leqslant \varepsilon_0^2$) for rings of fixed length $N$ we replace the condition (52) by the slightly weaker form:

$$\sqrt{N}\sqrt{\varepsilon_0^2} \ll 4\pi \tag{52a}$$

at the Fermi level of the half-filled band.

Finally, an important restriction on the allowed flux values in (49), (50*a*) and (50*b*) arises from the second-order perturbation expression for the effect of the disorder in the energy levels (9)–(11). This requires the typical second-order corrections of the energy levels to have magnitudes of the order of $\varepsilon_0^2$. In the half-filled band case this condition is generally obeyed by equations (39) and (40) for $\langle E_k^{(2)}\rangle$ at the Fermi level (where $\sin q_k \simeq 1$) by requiring $\cot\frac{2\pi\phi}{\phi_0} \simeq 1$. This yields a lower limit

$$\phi_{\min} = 0.125\phi_0, \tag{53}$$

for the flux values at which the perturbation treatment of the disorder is valid.

We close this subsection with some typical numerical results for the renormalization factor in (49), (50*a*) and (50*b*):

$$A = 1 - \frac{N\varepsilon_0^2(1-2\eta)}{8\sin^2\frac{2\pi\phi}{\phi_0}}, \qquad \eta = \frac{\alpha^2}{\varepsilon_0^2}, \tag{54}$$

of the pure system current by the effect of the disorder as a function of the correlation parameter $\eta = \alpha^2/\varepsilon_0^2$. We choose $|\varepsilon_0| = 0.1$ and define a typical ring length $N = (0, 4\pi)^2/\varepsilon_0^2 = 158$ compatible with (52*a*). Using these values, we obtain the results listed in table 1, for various values of $\eta$, for $\phi = \phi_{\min}$ and for an intermediate value, $\phi = 0.25\phi_0$, in the domain $0 < \phi/\phi_0 < 1/2$. Note that increasing the flux in the case $\eta < 0.5$ enhances the magnitude of the disorder effect on the persistent current, while in the case $\eta > 0.5$, increasing the flux reduces the effect of the correlated disorder.

**Table 1.** Disorder-dependent free-electron persistent current renormalization factor (53) for various values of the disorder correlation parameter $\eta$.

| $\eta$ | $\frac{\phi}{\phi_0}$ | $A$ |
|---|---|---|
| 0 | 0.125 | 0.605 |
| | 0.25 | 0.803 |
| 0.2 | 0.125 | 0.769 |
| | 0.25 | 0.882 |
| 0.4 | 0.125 | 0.921 |
| | 0.25 | 0.961 |
| 0.5 | — | 1 |
| 0.6 | 0.125 | 1.079 |
| | 0.25 | 1.040 |

## 4. Concluding remarks

The main conclusions of this work have been discussed in section 3 along with our detailed results for persistent currents in a metal ring in the presence of correlated disorder and the discussion of their domain of validity.

We conclude with some further general remarks, particularly in connection with the yet unexplained experimental observations of persistent currents.

By studying the persistent current in sufficiently large ensembles of rings it has been possible recently to obtain the correct sign, in addition to the magnitude, of the current [24–26]. These measurements have shown the persistent current to be diamagnetic at low fields (i.e. $\frac{d\langle I\rangle}{d\phi} < 0, \phi \to 0$). This observation constitutes a severe additional constraint for the validity of theoretical explanations of persistent current in disordered rings. Indeed, as shown by (16), (17*a*) and (17*b*), a diamagnetic persistent current for any parity of the number of conduction electrons is generally obtained only for non-interacting free electrons. Now, our analytical expressions (49), (50*a*) and (50*b*) for the effect of disorder on the persistent current in a half-filled band includes an additional flux dependence which prevents the current from having a fixed negative sign independent of parity and ring size. We observe, however, that our theoretical results for persistent currents are inapplicable to measurements in rings of mesoscale perimeters of 2–8 $\mu$m used in the various experimental studies [4–6] and [24–26]. Indeed, for values $|\varepsilon_0^2| \simeq 0.1$, with corresponding values $0 < |\alpha| \leqslant 0.1$, the condition (52) restricts the validity of our results to rings with a few hundred atomic sites, i.e. to nanoscale perimeters less than 100 nm. We note incidentally that typical ring sizes for which the effect of correlations of the random potential has been analysed numerically in [17–19] lie also in this range. In conclusion, it would be interesting if experimental studies could be performed for ensembles of rings of nanoscale sizes in order to test the detailed behaviour of persistent currents shown theoretically in this paper and numerically, for a different model, in [17–19].

Our results for the persistent current for a half-filled band in our ARDM model indicate a strong enhancement of the current due to the correlation of the random potential for $\alpha^2 \geqslant \varepsilon_0^2/2$. The detailed mechanism for the enhancement of persistent current by correlation for the ARDM model [11] on a ring threaded by a magnetic flux is quite different from the mechanism identified in recent numerical calculations for the RDM model of Dunlap, Wu and Phillips [12] in [17, 19]. We recall that the linear chain RDM model differs essentially from the ARDM by the existence of a fraction $\sqrt{N}$ of extended states [12, 13]. For the RDM model values of persistent current of the order of the values for free electrons are found only when the Fermi level coincides with the energy of an extended state, both for even $N_e$ [17, 19] and for odd $N_e$ (for an asymmetric dimer model) [18]. In contrast, for $N_e$ values corresponding to relatively large band fillings but for which the Fermi level does not coincide with an extended state, the persistent current is found to be strongly diminished by the correlated disorder [17, 18]. Thus for the RDM a strong compensation of the current reduction due to the uncorrelated disorder by the effect of correlation does not seem to exist [17, 18], in contrast to what is shown for the half-filled band in (49) (50*a*) and (50*b*) for the ARDM. We note, however, that the numerical results of [17, 18] pertain to a case of maximal disorder (equal number of *a* and *b* atoms in the RDM), while our analytical results are restricted to weak disorder in the ARDM.

As shown in section 3.3, our results for the persistent current are valid only for flux values larger than a value of the order of $\phi_0/8$. Thus the sign of the persistent current obtained from equations (49), (50*a*) and (50*b*) could be compared with experimental results at flux values $\phi > \phi_0/8$ only, rather than for $\phi \to 0$ as in recent experimental studies [24–26].

## Appendix

Defining

$$A_{n\,m} = \frac{\sin(n-m)q_k \sin(N-n+m)q_k}{\sin q_k \sin N\, q_k}, \qquad \text{(A.1)}$$

the various contributions to the disorder average, $\langle E_k^{(2)} \rangle$, of (11) are given by

$$\frac{1}{N}\sum_{n=2}^{N}\sum_{m=1}^{n-1}\langle (E^{(1)})^2\rangle A_{nm} = -\frac{(\varepsilon_0^2+\alpha^2)}{4N\sin q_k} \times (N\cot Nq_k - \cot q_k), \qquad \text{(A.2)}$$

$$\frac{1}{N}\sum_{n=2}^{N}\sum_{m=1}^{n-1}\langle \varepsilon_m\varepsilon_n\rangle A_{nm} = \frac{\alpha^2}{2}\frac{\sin(N-1)q_k}{\sin q_k}, \qquad \text{(A.3)}$$

$$\begin{aligned} -\frac{1}{N}\sum_{n=2}^{N}\sum_{m=1}^{n-1}\langle \varepsilon_m E^{(1)}\rangle A_{nm} &= \frac{(\varepsilon_0^2-\alpha^2)}{4N\sin q_k}(N\cot Nq_k - \cot q_k) \\ &+ \frac{\alpha^2}{4N^2\sin q_k \sin Nq_k}\Bigg\{N^2\cos Nq_k \\ &- 2\left[\frac{\mathrm{e}^{-\mathrm{i}(N+2)q_k}}{1-\mathrm{e}^{-4iq_k}}\left(\frac{\mathrm{e}^{4iq_k}(1-\mathrm{e}^{2\mathrm{i}Nq_k})}{1-\mathrm{e}^{4iq_k}} - \frac{N}{2}\right) + \text{c.c.}\right] \\ &- 2\left[\frac{\mathrm{e}^{-\mathrm{i}Nq_k}}{1-\mathrm{e}^{-4iq_k}}\left(\frac{1-\mathrm{e}^{2\mathrm{i}Nq_k}}{1-\mathrm{e}^{4iq_k}} - \frac{N}{2}\right) + \text{c.c.}\right]\Bigg\}, \end{aligned} \qquad \text{(A.4)}$$

$$\begin{aligned} -\frac{1}{N}\sum_{n=2}^{N}\sum_{m=1}^{n-1}\langle E^{(1)}\varepsilon_n\rangle A_{nm} &= \frac{(\varepsilon_0^2-\alpha^2)}{4N\sin q_k}(N\cot Nq_k - \cot q_k) \\ &+ \frac{\alpha^2}{4N^2\sin q_k \sin Nq_k}\Bigg\{2N(N-1)\cos Nq_k \\ &- \Bigg[\frac{\mathrm{e}^{-\mathrm{i}(N-2)q_k}}{1-\mathrm{e}^{-2iq_k}}\Bigg(\frac{1-\mathrm{e}^{2\mathrm{i}(N-1)q_k}}{1-\mathrm{e}^{2iq_k}} \\ &+ \frac{1+\mathrm{e}^{-2iq_k} - \mathrm{e}^{2\mathrm{i}Nq_k}(\mathrm{e}^{4iq_k}+\mathrm{e}^{-2iq_k})}{1-\mathrm{e}^{4iq_k}} \\ &- (N-1)\mathrm{e}^{2iq_k} - \left(\frac{N}{2}+1\right)\mathrm{e}^{-2iq_k} \\ &- \frac{N}{2}\mathrm{e}^{-6iq_k}\Bigg) + \text{c.c.}\Bigg]\Bigg\}. \end{aligned} \qquad \text{(A.5)}$$

The sum of (A.2)–(A.5) leads, after appropriate reductions, to the final form in (13)–(15).

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