Generalized waveguide approach to tight-binding wires: Understanding large vortex currents in quantum rings

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We generalize the quantum waveguide approach to Hückel or tight-binding models relevant to unsaturated π molecular devices. A Landauer-type formula for the current density through *internal* bonds is also derived which allows for defining a local conductance. The approach is employed to study internal circular currents in two-terminal rings. We show how to predict the occurrence and the nature of large vortex currents in coincidence with vanishingly small currents in the leads. We also prove a remarkably simple formula for the onset of a vortex regime.

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I. INTRODUCTION

The quantum waveguide approach (WGA) introduced in Refs. 1 and 2 has been extensively used to study multiterminal mesoscopic structures, such as quantum rings or quantum wires, possibly in the presence of impurities, magnetic fields, Rashba interactions, or Dresselhaus interactions. The basic idea of the WGA is to calculate the one-particle wave function $\varphi_n(x)=a_n e^{ikx}+b_n e^{-ikx}$ in the nth wire by imposing the continuity at each vertex, i.e., $\varphi_1(0)=\varphi_2(0)=\cdots=\varphi_{\mathcal{N}}(0)$ ($\mathcal{N}$ is the number of intersecting wires at the vertex), and the additional condition $\Sigma_{n=1}^{\mathcal{N}}\varphi_n'(0)=0$, which implies current conservation at the vertex (the derivative is taken along the incoming direction). It is worth noticing that current conservation is actually fulfilled by the weaker condition

$$\sum_{n=1}^{\mathcal{N}} \varphi_n'(0) = r\varphi_1(0), \tag{1}$$

where r is an arbitrary real number. To our knowledge such arbitrariness has never been discussed.

In recent years it became possible to attach aromatic molecules or atomic chains to leads. These structures are geometrically similar to their mesoscopic counterparts and call for a Hückel-type or tight-binding (TB) generalization of the WGA due to the inadequacy of the continuum free-particle description. In the discrete case the difficulty stems from the fact that we cannot impose a condition on the derivative of the wave function. Approaches based on the Green's functions,[3] iterative procedures,[4] or source-and-sink potentials[5,6] have been proposed but none of them is directly related to the WGA.

It is the purpose of this work to show how to generalize the WGA to the TB case (TBWGA) and to use the method to predict the occurrence of large vortex currents in quantum rings observed for the first time in Ref. 4. The continuum case is recovered by a proper limit of the TB parameters and allows us to understand the physical meaning of the real constant r in Eq. (1).

II. TIGHT-BINDING WGA

We consider a generic system consisting of TB chains with at least one endpoint in common. In Fig. 1 we illustrate a vertex of the system with $\mathcal{N}=4$ intersecting chains. Let ε_n be the onsite energy of the nth chain, t_n be the hopping parameter between the nearest-neighbor sites, and ε_V be the onsite energy of the vertex. We denote with $\psi_{\varepsilon n}(j)=a_{\varepsilon n}e^{ik_n j}+b_{\varepsilon n}e^{-ik_n j}$ the amplitude on the jth site of the nth chain of an eigenstate of energy $\varepsilon=\varepsilon_n+2t_n\cos k_n$. As in the continuum case the continuity of the wave function yields $\mathcal{N}-1$ independent equations,

$$\psi_{\varepsilon 1}(0) = \psi_{\varepsilon 2}(0) = \cdots = \psi_{\varepsilon \mathcal{N}}(0). \tag{2}$$

The additional condition, which plays the role of Eq. (1) in the WGA, is obtained by projecting on the vertex site the stationary Schrödinger equation

$$\sum_{n=1}^{\mathcal{N}} t_n\psi_{\varepsilon n}(1) + \varepsilon_V\psi_{\varepsilon 1}(0) = \varepsilon\psi_{\varepsilon 1}(0). \tag{3}$$

Equations (2) and (3) provide $\mathcal{N}$ independent equations for each vertex of the system. Thus, for a system having $\mathcal{V}$ vertices with $\mathcal{N}_i$, $i=1,\ldots,\mathcal{V}$, intersecting chains at the ith vertex, the above procedure yields $\Sigma_i\mathcal{N}_i$ equations. Letting $\mathcal{P}$ be the number of chains with both endpoints belonging to the set of vertices and $\mathcal{Q}$ be the number of semi-infinite chains with one endpoint connected to a vertex, i.e., the number of terminals, we have $2\mathcal{P}+\mathcal{Q}=\Sigma_i\mathcal{N}_i$ and hence a degeneracy $D\leq\mathcal{Q}$ for each energy level (the number of unknown constants $\{a_{\varepsilon n}\}$ and $\{b_{\varepsilon n}\}$ is $2\mathcal{P}+\mathcal{Q}+D$ where D is the number of terminals for which $|\varepsilon-\varepsilon_n|<2|t_n|$), as should be.

To recover the WGA we employ a three-point discretization of the kinetic term (our argument does not rely on this specific way of discretizing). Then, $t_n=-1/(2\Delta^2)$ and $\varepsilon_n=1/\Delta^2$, where Δ is the spacing between two points of the continuum wire (we use atomic units). The amplitudes $\psi_{\varepsilon n}(1)$ correspond to the amplitudes of the wave function at

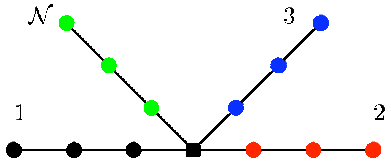

FIG. 1. (Color online) Illustration of a vertex with $\mathcal{N}=4$.

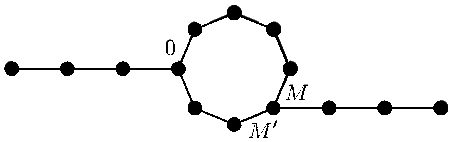

FIG. 2. Illustration of a ring device with $M=5$ and $N=8$. The last site of the lower arm is $M'=N-M$.

a distance Δ from the vertex. For clarity we then rename $\psi_{\varepsilon n}(j)$ with $\psi_{\varepsilon n}(j\Delta)$ and rewrite Eq. (3) as

$$\sum_{n=1}^{\mathcal{N}} \left[\frac{\psi_{\varepsilon n}(\Delta) - \psi_{\varepsilon n}(0)}{\Delta} \right] - \Delta \tilde{\varepsilon}_V \psi_{\varepsilon 1}(0) = -2\varepsilon\Delta\psi_{\varepsilon 1}(0), \quad (4)$$

where $\tilde{\varepsilon}_V \equiv 2\varepsilon_V - \mathcal{N}/\Delta^2$. Taking the continuum limit $\Delta \to 0$ we recover Eq. (1) provided that $\lim_{\Delta\to 0} \Delta\tilde{\varepsilon}_V = r$, which implies $\tilde{\varepsilon}_V \sim r/\Delta$. Thus, the constant r is the amplitude of the δ-like potential $r\delta(x)$ at the vertex and is zero only for smooth potentials.

III. TWO-TERMINAL SYSTEMS

We now focus on two-terminal systems and obtain a *Landauer-type formula for the current density through a generic bond*. Let $H^{(0)} = H_{\text{leads}} + H_{\text{dev}} + H_{\text{tun}}$ be the Hamiltonian of the system in equilibrium. The Hamiltonian of the left (L) and right (R) leads is

$$H_{\text{leads}} = t\sum_{j<0} (c_j^\dagger c_{j-1} + \text{H.c.}) + t\sum_{j>0} (c_j^\dagger c_{j+1} + \text{H.c.}), \quad (5)$$

with nearest-neighbor hopping t. The device is described by $H_{\text{dev}} = \Sigma_{nm=1}^{N} t_{nm} d_n^\dagger d_m$ with real parameters $t_{nm} = t_{mn}$ and N is the total number of sites. The device is connected to the left lead through site 1 and to the right lead through site $M \leq N$ (see, e.g., Fig. 2). The tunneling Hamiltonian is

$$H_{\text{tun}} = t_L(d_1^\dagger c_{-1} + \text{H.c.}) + t_R(d_M^\dagger c_1 + \text{H.c.}). \quad (6)$$

We are interested in the long-time limit of the current density when an external bias U_α is imposed on lead $\alpha = L, R$.[7]

At zero temperature the long-time limit of the density matrix $\rho_{x,x'}$, with x, x' site indices of either the leads or the device, is given by the sum of a steady-state contribution $\rho^{(S)}_{x,x'}$ and a dynamical contribution.[8] The steady-state contribution can be written in terms of left-going eigenstates $|\psi_{\varepsilon R}\rangle$ and right-going eigenstates $|\psi_{\varepsilon L}\rangle$ as

$$\rho^{(S)}_{x,x'} = \sum_{\alpha=L,R} \int_{-2|t|+U_\alpha}^{\varepsilon_F+U_\alpha} \frac{d\varepsilon}{2\pi} \psi_{\varepsilon\alpha}(x')\psi^*_{\varepsilon\alpha}(x), \quad (7)$$

with ε_F as the equilibrium Fermi energy. The states are normalized according to $\langle \psi_{\varepsilon\alpha} | \psi_{\varepsilon'\beta} \rangle = 2\pi\delta_{\alpha\beta}\delta(\varepsilon - \varepsilon')$. Without loss of generality we choose $U_L > U_R$ and split Eq. (7) into three terms containing the contribution of the left-going evanescent states with energy in the range $(-2|t| + U_R, -2|t| + U_L)$, the left- and right-going current-carrying states with energy in the range $(-2|t| + U_L, \varepsilon_F + U_R)$, and the right-going current-carrying states with energy in the range $(\varepsilon_F + U_R, \varepsilon_F + U_L)$. The evanescent states can be chosen real valued since they are nondegenerate and the biased Hamiltonian is invariant under time reversal. Thus, the imaginary part of $\rho^{(S)}_{x,x'}$ simplifies to

$$\Im[\rho^{(S)}_{x,x'}] = \int_{\varepsilon_F+U_R}^{\varepsilon_F+U_L} \frac{d\varepsilon}{2\pi} \Im[\psi_{\varepsilon L}(x')\psi^*_{\varepsilon L}(x)] + \int_{-2|t|+U_L}^{\varepsilon_F+U_R} \frac{d\varepsilon}{2\pi} \sum_\alpha \Im[\psi_{\varepsilon\alpha}(x')\psi^*_{\varepsilon\alpha}(x)]. \quad (8)$$

Let us first consider the case in which both x, x' are site indices of the same lead. The amplitude on the leads $\psi_{\varepsilon\alpha}(j) \equiv \langle 0|c_j|\psi_{\varepsilon\alpha}\rangle$ of a normalized scattering state is

$$\psi_{\varepsilon L}(j) = \sqrt{\nu_L(\varepsilon)} \begin{cases} e^{iqj} + R_{\varepsilon L} e^{-iqj}, & j < 0 \\ T_{\varepsilon L} e^{i\tilde{q}j}, & j > 0, \end{cases} \quad (9)$$

$$\psi_{\varepsilon R}(j) = \sqrt{\nu_R(\varepsilon)} \begin{cases} T_{\varepsilon R} e^{-iqj}, & j < 0 \\ e^{-i\tilde{q}j} + R_{\varepsilon R} e^{i\tilde{q}j}, & j > 0, \end{cases} \quad (10)$$

with $\varepsilon = 2t\cos(q) + U_L = 2t\cos(\tilde{q}) + U_R$ and $\nu_\alpha(\varepsilon) = 1/\sqrt{4t^2 - (\varepsilon - U_\alpha)^2}$ is the density of states in lead α. Exploiting current conservation and the orthogonality condition between left- and right-going eigenstates, i.e., $R^*_{\varepsilon L} T_{\varepsilon R}/\nu_L(\varepsilon) + R_{\varepsilon R} T^*_{\varepsilon L}/\nu_R(\varepsilon) = 0$, it is straightforward to show that for $x = j > 0$ and $x' = j+1$ the second term in Eq. (8) vanishes while the first term reduces to the well-known Landauer formula

$$\Im[\rho^{(S)}_{j,j+1}] = \frac{1}{2|t|} \int_{\varepsilon_F+U_R}^{\varepsilon_F+U_L} \frac{d\varepsilon}{2\pi} |T_{\varepsilon L}|^2 \frac{\nu_L(\varepsilon)}{\nu_R(\varepsilon)}. \quad (11)$$

Below we show that the possibility of expressing $\Im[\rho^{(S)}_{x,x'}]$ as an integral over the bias window is valid *for all sites* including those in the central device. Let us express $\psi_{\varepsilon R}$ as a linear combination of $\psi_{\varepsilon\alpha}$ and the time-reversal state $\psi^T_{\varepsilon\alpha} = \psi^*_{\varepsilon\alpha}$,

$$\psi_{\varepsilon R}(x) = \sqrt{\frac{\nu_R(\varepsilon)}{\nu_L(\varepsilon)}} \frac{1}{T^*_{\varepsilon L}} [\psi^*_{\varepsilon L}(x) - R^*_{\varepsilon L}\psi_{\varepsilon L}(x)]. \quad (12)$$

Extracting the transmission and reflection coefficients $T_{\varepsilon R}$ and $R_{\varepsilon R}$, one can easily verify that $\psi_{\varepsilon R}(x)$ is orthogonal to $\psi_{\varepsilon L}(x)$. Inserting Eq. (12) into Eq. (8) and exploiting current conservation for the right-going scattering state, one realizes that the imaginary part of $\Sigma_\alpha \psi_{\varepsilon\alpha}(x')\psi^*_{\varepsilon\alpha}(x)$ is identically zero, and hence only states in the bias window contribute to $\Im[\rho^{(S)}_{x,x'}]$. Thus, the long-time limit of the current density $J_{nm} \equiv 2t_{nm}\Im[\rho^{(S)}_{n,m}]$ through an internal bond of the device connecting site n to site m can be expressed in a Landauer-type formula. In linear response $J_{nm} = G_{nm}(U_L - U_R)$ and exploiting the above result, the *local conductance* G_{nm} is given by

$$G_{nm} \equiv \frac{J_{nm}}{U_L - U_R} = \frac{t_{nm}}{\pi} \Im[\psi_{\varepsilon_F L}(m)\psi^*_{\varepsilon_F L}(n)]. \quad (13)$$

We next specialize the analysis to devices consisting of a TB ring and address the existence of vortex regimes.

IV. CONDUCTANCES IN TWO-TERMINAL RINGS

We consider a ring with N sites, see Fig. 2. For notational convenience we denote with $d_{\Uparrow n}$, $n = 0, \ldots, M$, the fermionic operators in the upper arm and with $d_{\Downarrow n}$, $n = 0, \ldots, N-M$, the

fermionic operators in the lower arm, and we identify $d_{\Uparrow 0} \equiv d_{\Downarrow 0}$ and $d_{\Uparrow M} \equiv d_{\Downarrow N-M}$. In terms of the operators $d_{\Uparrow n}, d_{\Downarrow n}$ the device Hamiltonian reads

$$H_{\rm dev} = t\sum_{n=0}^{M-1} (d_{\Uparrow n}^{\dagger} d_{\Uparrow n+1} + \text{H.c.}) + t\sum_{n=0}^{M'-1} (d_{\Downarrow n}^{\dagger} d_{\Downarrow n+1} + \text{H.c.}), \quad (14)$$

where $M' = N - M$ and the hopping t is the same as in the leads. For simplicity we also set $t_L = t_R = t$ in the tunneling Hamiltonian. We employ the TBWGA to calculate, e.g., the right-going eigenstates $\psi_{\varepsilon L}$. Let $\psi_{\varepsilon L}(j) = \sqrt{\nu_L(\varepsilon)}(e^{ikj} + R_{\varepsilon L} e^{-ikj})$ be the amplitude on lead L $(j \le 0)$ and $\psi_{\varepsilon L}(j) = \sqrt{\nu_L(\varepsilon)} T_{\varepsilon L} e^{ikj}$ be the amplitude on lead R $(j \ge 0)$. Similarly, the wave function on the upper arm of the ring has the form $\psi_{\varepsilon L}(n) = \sqrt{\nu_L(\varepsilon)}(A_{\varepsilon L} e^{ikn} + B_{\varepsilon L} e^{-ikn})$ with $0 \le n \le M$ while on the lower arm $\psi_{\varepsilon L}(n) = \sqrt{\nu_L(\varepsilon)}(C_{\varepsilon L} e^{ikn} + D_{\varepsilon L} e^{-ikn})$ with $0 \le n \le N - M$. According to the TBWGA the coefficients of $\psi_{\varepsilon L}$ are solution of

$$\begin{pmatrix} 1 & 1 & 0 & 0 & -1 & 0 \\ 0 & 0 & 1 & 1 & -1 & 0 \\ e^{ikM} & e^{-ikM} & 0 & 0 & 0 & -1 \\ 0 & 0 & e^{ik(N-M)} & e^{-ik(N-M)} & 0 & -1 \\ e^{ik} & e^{-ik} & e^{ik} & e^{-ik} & -e^{-ik} & 0 \\ e^{ik(M-1)} & e^{-ik(M-1)} & e^{ik(N-M-1)} & e^{-ik(N-M-1)} & 0 & -e^{-ik} \end{pmatrix} \begin{pmatrix} A_{\varepsilon L} \\ B_{\varepsilon L} \\ C_{\varepsilon L} \\ D_{\varepsilon L} \\ R_{\varepsilon L} \\ T_{\varepsilon L} \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \\ e^{ik} \\ 0 \end{pmatrix}. \quad (15)$$

Left-going states $\psi_{\varepsilon R}$ can be computed in a similar manner and it is straightforward to show that $T_{\varepsilon L} = T_{\varepsilon R} \equiv T_{\varepsilon}$, which is the transmittance of the system. The conductance through a bond is given by Eq. (13). For any bond in the leads the conductance is simply $G_{\varepsilon} = |T_{\varepsilon}|^2 g_0$, where $g_0 = 1/(2\pi)$ is the quantum of conductance for spinless electrons. The conductances on the upper and lower arms of the ring are $G_{\Uparrow \varepsilon} = (|A_{\varepsilon L}|^2 - |B_{\varepsilon L}|^2) g_0$ and $G_{\Downarrow \varepsilon} = (|C_{\varepsilon L}|^2 - |D_{\varepsilon L}|^2) g_0$. From the above system of equations we obtain the following analytical solution for the transmittance and the local conductance:

$$T_{\varepsilon} = \frac{i e^{ik(2M-N)} \sin^2(k) \sin\left(k\frac{N}{2}\right) \cos\left[k\left(\frac{N}{2} - M\right)\right]}{\Omega(k)}, \quad (16)$$

$$\frac{G_{\Uparrow \varepsilon}}{g_0} = \frac{\sin^4(k) \sin\left(k\frac{N}{2}\right) \cos\left[k\left(\frac{N}{2} - M\right)\right] \sin[k(N-M)]}{2|\Omega(k)|^2}, \quad (17)$$

$$\frac{G_{\Downarrow \varepsilon}}{g_0} = \frac{\sin^4(k) \sin\left(k\frac{N}{2}\right) \cos\left[k\left(\frac{N}{2} - M\right)\right] \sin(kM)}{2|\Omega(k)|^2}, \quad (18)$$

with

$$\Omega(k) = \frac{e^{-2ik(N-M+2)}}{16}[1 - 4e^{2ik}(1 - e^{2ik}) - e^{2ik(M+2)} + e^{2ikN} - 2e^{ikN}(e^{2ik} - 1)^2 - e^{2ik(N-M+2)}]. \quad (19)$$

It is easy to verify that current conservation is fulfilled since $G_{\Uparrow \varepsilon} + G_{\Downarrow \varepsilon} = |T_{\varepsilon}|^2 g_0 = G_{\varepsilon}$. It is also worth emphasizing that G_{ε} is bounded between 0 and g_0, while $G_{\Uparrow \varepsilon}$ and $G_{\Downarrow \varepsilon}$ can be much larger than g_0 and can be either positive or negative. We say that we are in a *vortex regime* if $\text{sign}[G_{\Uparrow \varepsilon}] = -\text{sign}[G_{\Downarrow \varepsilon}]$. From Eqs. (17) and (18) we conclude that *for arms of different length a vortex regime always exists* since

$$\frac{G_{\Uparrow \varepsilon}}{G_{\Downarrow \varepsilon}} = \frac{\sin[k(N-M)]}{\sin(kM)}. \quad (20)$$

Equation (20) is simple and transparent. The onset of a vortex occurs for those values of the incident momentum corresponding to an eigenenergy of either the isolated lower arm $k_n^{(\mathcal{L})} = \pi n/(N-M)$ or the isolated upper arm $k_m^{(\mathcal{U})} = \pi m/M$. In the following we characterize the vortex regime and show how to predict the occurrence of large ring currents in coincidence with a vanishingly small current in the leads.

V. VORTEX REGIME

As already pointed out in Refs. 6 and 9 the transmittance T_{ε} has two different kinds of zeros. The numerator in Eq. (16) vanishes either for energies that exactly match an eigenvalue of the isolated ring, i.e., for $k_n^{(\mathcal{M})} = 2n\pi/N$ (*matching momenta*), or for energies at which there is perfect destructive interference at the right interface, i.e., for $k_m^{(\mathcal{I})} = (2m+1)\pi/(N-2M)$ (*interference momenta*). At these points the transmittance vanishes provided the denominator $\Omega(k) \neq 0$. From the linear system in Eq. (15) one can easily show that $\Omega(k)$ cannot be zero at the interference momenta since the wave function at the right interface vanishes and hence T_{ε} vanishes as well. As the numerator of T_{ε} goes to zero as $\sim(k - k_n^{(\mathcal{I})})$ the denominator $\Omega(k)$ has to be finite. On the other hand, the denominator can vanish at the matching momenta for special values of M/N. Expanding $\Omega(k)$ around $k_n^{(\mathcal{M})}$ one finds to the first order $\Omega(k) \approx -(e^{4iMn\pi/N} - 1)^2/16 + \gamma(n)(k - k_n^{(\mathcal{M})})$, with $|\gamma(n)| > \sqrt{N(2N-3) + M(4N+2)} > 0$. Thus $\Omega(k)$ approaches zero as $(k - k_n^{(\mathcal{M})})$ for integer $2Mn/N$. In these cases the simple zero of the denominator cancels the simple zero of the numerator and T_{ε} is finite (unless $k_n^{(\mathcal{M})}$ is

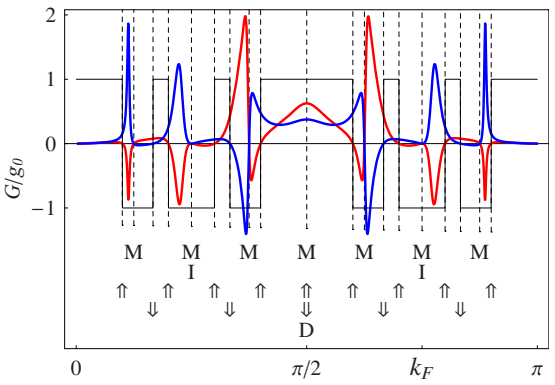

FIG. 3. (Color online) Local conductance $G_{\Uparrow\varepsilon}/g_0$ (red), $G_{\Downarrow\varepsilon}/g_0$ (blue), and $S_\varepsilon \equiv \mathrm{sign}\{\sin[k(N-M)]/\sin(kM)\}$ (black), see Eq. (20), versus the incident momentum k for $N=16$ and $M=6$. The function S_ε is 1 in the laminar regime and −1 in the vortex regime. Vertical dashed lines are drawn in correspondence of $k=k^{\mathcal{M}}$ (M), $k=k^{\mathcal{I}}$ (I), $k=k^{\mathcal{L}}$ ($\Uparrow$), $k=k^{\mathcal{U}}$ ($\Downarrow$), and of the zeros of $\Omega(k)$ (D).

an interference momentum as well). Our condition for the cancellation of zeros include the symmetric case $M=N/2$ already discussed in Ref. 9 as well as other cases, see Fig. 3 where $N=16$ and $M=6$ and the zero at $\pi/2$ is cancelled by the denominator (the conductance G_ε has the same zeros as the transmittance since $G_\varepsilon/g_0=|T_\varepsilon|^2$).

From Eqs. (17) and (18) one can see that a zero of G_ε implies a zero of both $G_{\Uparrow\varepsilon}$ and $G_{\Downarrow\varepsilon}$. Novel zeros, however, exist for the local conductances. Specifically, the numerator of $G_{\Uparrow\varepsilon}$ vanishes for $k=k_n^{(\mathcal{L})}$ while the numerator of $G_{\Downarrow\varepsilon}$ vanishes for $k=k_m^{(\mathcal{U})}$, see Fig. 3. Thus, the conductance $G_{\Uparrow\varepsilon}$ is zero at $k=k_n^{(\mathcal{L})}$ unless $k_n^{(\mathcal{L})}$ is also a zero of the denominator. In the latter case $G_{\Uparrow\varepsilon}$ remains finite since there exists an integer m such that $k_n^{(\mathcal{L})}=k_m^{(\mathcal{M})}$ and hence $\sin(Nk/2)\sin[k(N-M)]\sim[k-k_m^{(\mathcal{M})}]^2$ which cancels the double zero of $|\Omega(k)|^2$.[10] In Fig. 3 this cancellation takes place at $k=\pi/2$. A similar reasoning applies to $G_{\Downarrow\varepsilon}$. To summarize, the local conductances $G_{\Uparrow\varepsilon}$ and $G_{\Downarrow\varepsilon}$ as well as the transmittance T_ε can have simple or double zeros while G_ε can have double or quadruple zeros.

In accordance with the above analysis the onset of the vortex phase occurs for incident momenta $k=k^{(\mathcal{U})}\neq k^{(\mathcal{L})}$ or $k=k^{(\mathcal{L})}\neq k^{(\mathcal{U})}$. Below we show that in the vortex regime there are special values of the incident momentum yielding a circular ring current much larger than the current in the leads. In order to quantify this effect we define the vortex function

$$V(\varepsilon)=\frac{G_{\Uparrow\varepsilon}-G_{\Downarrow\varepsilon}}{G_\varepsilon}. \tag{21}$$

The modulus of $V(\varepsilon)$ is in the range (0,1) when $G_{\Uparrow\varepsilon}$ and $G_{\Downarrow\varepsilon}$ have the same sign (laminar regime) and is greater than one in the vortex regime. At the onset either $G_{\Uparrow\varepsilon}$ or $G_{\Downarrow\varepsilon}$ vanishes and $|V(\varepsilon)|=1$. The vortex function diverges at the zeros of the total conductance and the magnitude of the vortex can be classified according to the nature of zeros of G_ε. For double zeros of G_ε (single zeros of T_ε) the difference $G_{\Uparrow\varepsilon}-G_{\Downarrow\varepsilon}$ has a single zero since a double zero would imply $k^{(\mathcal{U})}=k^{(\mathcal{L})}$ which in turn implies $\Omega(k)=0$. Expanding the conductances around the single zero ε_s of T_ε, we find $V(\varepsilon)\sim 1/(\varepsilon-\varepsilon_s)$. The current flowing in the ring changes direction as ε crosses ε_s. It is worth noting that in the neighborhood of ε_s the derivative $G'_{\Uparrow/\Downarrow\varepsilon}$ can be very large (see Fig. 3 at $k_F=3\pi/8$) and $|G_{\Uparrow/\Downarrow\varepsilon}|\sim g_0 \gg G_\varepsilon \sim 10^{-1}g_0$. Even more striking is the behavior of $V(\varepsilon)$ around a double zero ε_d of T_ε. In this case $G_{\Uparrow\varepsilon}-G_{\Downarrow\varepsilon}$ also has a double zero[10] and hence $V(\varepsilon)\sim 1/(\varepsilon-\varepsilon_d)^2$. In this case the vortex does not change sign as ε crosses ε_d. Both divergences are rather remarkable since one could naively expect that $|G_{\Uparrow/\Downarrow\varepsilon}|<G_\varepsilon$ in accordance with Kirchoff's current laws of classical electromagnetism.

We also explored the vortex regime for nonzero onsite energies $\varepsilon_{\mathrm{dev}}$ on the ring and different couplings $t_{L/R}$. Varying $t_{L/R}$ alters the shape of $G_{\Uparrow/\Downarrow}$ but preserves both the position and the nature of the zeros. On the contrary, the position of the zeros changes as $\varepsilon_{\mathrm{dev}}$ is varied but a vortex regime still exists.

In conclusion we have generalized the WGA to TB models and obtained a Landauer-type formula for the current density through a generic bond. The TBWGA requires the *same* computational effort as the WGA. Employing the TBWGA in combination with the obtained expression of the local conductance, we have shown how to predict the occurrence of large vortex currents. The existence of a vortex regime is rather robust and has to be attributed to the nontrivial topology of the system rather than to a specific choice of the parameters.

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[10] The conclusion that the local conductance in the rings remains finite relies on the fact that it is not possible to have a triple zero in the numerator of Eqs. (17) and (18), i.e., it is not possible to verify $k^{(\mathcal{M})}=k^{(\mathcal{I})}=k^{(\mathcal{U}/\mathcal{L})}$.