Transmission through two-dimensional tight-binding lattices

B. L. Burrows
Mathematics Section, School of Computing, Staffordshire University, Beaconside, Stafford ST18 0DG, United Kingdom

K. W. Sulston
Department of Mathematics and Computer Science, University of Prince Edward Island, Charlottetown, Prince Edward Island, Canada C1A 4P3

(Received 1 June 1999; revised manuscript received 8 March 2000)

A methodology of transmission through two-dimensional tight-binding lattices is presented. The theory is formulated in terms of matrix algebra and the relationships between the matrices are examined in detail. The features specific to tight-binding systems are contrasted to those for more general transmission problems. Illustrative examples are given to indicate the wide applicability of the methodology.

I. INTRODUCTION

We consider here the problem of two-dimensional transmission through a material B, which forms part of a larger composite system, by ''sandwiching'' B between the other two components A_l and A_r (which may be the same material); i.e., we have the system represented by A_l-B-A_r. We are not specific about the composition of the materials or the identity of the transmitted particle, as the formalism is general enough to treat a variety of different situations. For example, possible applications include electronic transmission through a Penrose tiling[1–3] or Fibonacci lattice,[4] possibly in the presence of a magnetic field.[5] Other possibilities involve the generalization of previous one-dimensional work on neutron or atom polarization through periodic[6] or quasiperiodic[7,8] magnetic lattices. In the work presented here we confine ourselves to the case where A_l and A_r are the same material.

For a stationary state of the composite system, with definite energy E, the transmission through any part of the system must be conserved. The measure of transmission used here is a direct analogy with the widely used definition for one-dimensional problems, but in certain examples, particularly where the transmission is small, this necessitates very high precision. This is considered in detail in the Appendix where the reasons are elucidated, but the calculations presented here are sufficiently precise to overcome this problem. Since transmission is an important property for the stationary states of the composite systems considered, we have chosen to calculate this directly, rather than to use other measures which average over different channels corresponding to different energies and consequently to different stationary states.

II. GENERAL THEORY

For a stationary state of the composite system it is required that the current through B be conserved. The general problem of multichannel scattering has been considered by Imry,[9] and can be represented schematically as in Fig. 1. The vector $\mathbf{a}_l(\mathbf{b}_r)$ contains the amplitudes of the incoming channels from the left (right) and similarly $\mathbf{b}_l(\mathbf{a}_r)$ those of outgoing channels to the left(right). These vectors are related by the equation

$$\begin{pmatrix}\mathbf{a}_r\\ \mathbf{b}_r\end{pmatrix}=T\begin{pmatrix}\mathbf{a}_l\\ \mathbf{b}_l\end{pmatrix}=\begin{pmatrix}T_1 & T_2\\ T_3 & T_4\end{pmatrix}\begin{pmatrix}\mathbf{a}_l\\ \mathbf{b}_l\end{pmatrix}, \tag{1}$$

where T is the transfer matrix and current conservation implies that

$$\mathbf{a}_l^+\mathbf{a}_l-\mathbf{b}_l^+\mathbf{b}_l=\mathbf{a}_r^+\mathbf{a}_r-\mathbf{b}_r^+\mathbf{b}_r. \tag{2}$$

Equation (1) can be regarded as defining $\mathbf{a}_r$ and $\mathbf{b}_r$ in terms of $\mathbf{a}_l$ and $\mathbf{b}_l$. If Eq. (2) is to hold for all vectors satisfying Eq. (1), then certain conditions must hold. By writing the right hand side of Eq. (2) in terms of $\mathbf{a}_l$ and $\mathbf{b}_l$ we see that the appropriate conditions on the submatrices in T are

$$\begin{aligned}(T_1^+T_1-T_3^+T_3)&=I=(T_4^+T_4-T_2^+T_2),\\ (T_2^+T_1-T_4^+T_3)&=0=(T_1^+T_2-T_3^+T_4).\end{aligned} \tag{3}$$

Putting Eq. (3) into matrix form gives

$$\begin{aligned}\begin{pmatrix}T_1^+ & -T_3^+\\ -T_2^+ & T_4^+\end{pmatrix}\begin{pmatrix}T_1 & T_2\\ T_3 & T_4\end{pmatrix}&=\begin{pmatrix}I & 0\\ 0 & I\end{pmatrix}\\ &=\begin{pmatrix}T_1 & T_2\\ T_3 & T_4\end{pmatrix}\begin{pmatrix}T_1^+ & -T_3^+\\ -T_2^+ & T_4^+\end{pmatrix}.\end{aligned} \tag{4}$$

The right-hand side of Eq. (4) leads to the additional conditions

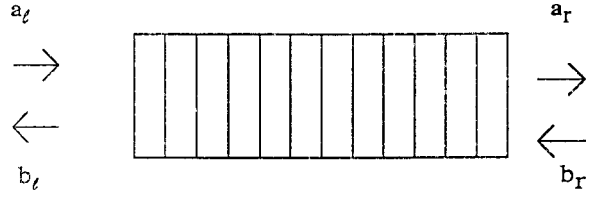

FIG. 1. A schematic diagram of two-dimensional scattering through subsystem B.

$$(T_1T_1^+ - T_2T_2^+) = I = (T_4T_4^+ - T_3T_3^+),$$

$$(T_2T_4^+ - T_1T_3^+) = 0 = (T_3T_1^+ - T_4T_2^+). \quad (5)$$

Equations (5) have also been derived (but in a different way) by Imry[9] and Pichard.[10] Specializing to the case where we only have outgoing amplitudes on the right-hand side, i.e., $\mathbf{b}_r = \mathbf{0}$, Eq. (1) leads to

$$\mathbf{b}_l = -T_4^{-1}T_3\mathbf{a}_l = r\mathbf{a}_l \quad (6)$$

and

$$\mathbf{a}_r = (T_1 - T_2T_4^{-1}T_3)\mathbf{a}_l = t\mathbf{a}_l, \quad (7)$$

where the matrices r and t are called the reflection and transmission matrices, respectively. Equation (2) reduces to the normalization condition

$$\mathbf{a}_l^+\mathbf{a}_l = \mathbf{a}_r^+\mathbf{a}_r + \mathbf{b}_l^+\mathbf{b}_l. \quad (8)$$

Using Eqs. (6)–(8) together motivates the definitions of transmission and reflection coefficients, namely,

$$\tau = \frac{\mathbf{a}_l^+ t^+ t\mathbf{a}_l}{\mathbf{a}_l^+\mathbf{a}_l}, \quad (9)$$

$$\rho = \frac{\mathbf{a}_l^+ + r\mathbf{a}_l}{\mathbf{a}_l^+\mathbf{a}_l} \quad (10)$$

with $\tau + \rho = 1$. We note as an aside that the relations (3) and (5) can be used to rewrite the transmission matrix as

$$t = (T_1^+)^{-1}. \quad (11)$$

III. TIGHT-BINDING TRANSMISSION

We now look at the situation of specific interest here, namely, two-dimensional tight-binding systems. The details of the analysis of the tight-binding systems used for A_l, B, and A_r are given in the Appendix, but essentially we take each subsystem to be finite, of length N in the y direction and B also to be finite of length M in the x direction. The atoms are numbered so that the atoms of B make up a rectangular array $m = 1 \cdots M$, $n = 1 \cdots N$. We take the subsystem A_l to be periodic in the x direction $m < 1$ and similarly A_r periodic in the x direction $m > M$. The assumptions outlined in the Appendix lead to wave function coefficients for the subsystem A_l in the form

$$c(m,n) = \sin(n\phi)(e^{im\theta} + B_n e^{-im\theta}), \quad m \leqslant 0 \quad (12)$$

for some real θ and ϕ, whose values are restricted by the boundary conditions, and the assumption of outgoing waves in the subsystem A_r leads to a similar form:

$$c(m,n) = \sin(n\phi)D_n e^{im\theta}, \quad m > M. \quad (13)$$

Writing $u_n = D_n e^{i(M+2)\theta}$ and combining the u_n and the B_n in vectors $\mathbf{u}$ and $\mathbf{B}$, respectively, we deduce in the Appendix that

$$\begin{pmatrix} \mathbf{u} \\ \mathbf{0} \end{pmatrix} = P \begin{pmatrix} \mathbf{1} \\ \mathbf{B} \end{pmatrix} \quad (14)$$

with

$$P = S_1^{-1}Q^{-1}\mathbf{R}QS_1, \quad (15)$$

where the matrix $\mathbf{R}$ connects the coefficients of the wave function at the two interfaces of subsystem B with the other subsystems,

$$Q = \begin{pmatrix} I & I \\ Ie^{-i\theta} & Ie^{i\theta} \end{pmatrix}, \quad (16)$$

$$S_1 = \begin{pmatrix} S & 0 \\ 0 & S \end{pmatrix}, \quad (17)$$

and S is a diagonal matrix whose (n,n) element is $\sin(n\phi)$.

A casual comparison of Eq. (14) with Eq. (1) might suggest that P acts as a transfer matrix that satisfies relations (3) and (5), and that $\mathbf{u}$ and $\mathbf{B}$ obey a current conservation law of the form of Eq. (2). But surprisingly this is not the case. The reason for this lies in the form of the tight-binding coefficients and specifically the presence of the $\sin(n\phi)$ factors therein. This affects the incoming and outgoing currents in subsystem B. Specifically, the outgoing current on the right is constructed from Eq. (13) as a sum of terms of the form $\sin^2(n\phi)|u_n|^2$. Similarly, the incoming and outgoing currents on the left are constructed from Eq. (12) as sums of terms $\sin^2(n\phi)$ and $\sin^2(n\phi)|B_n|^2$, respectively; i.e.,

$$\sum_n \sin^2(n\phi)|u_n|^2 = \sum_n \sin^2(n\phi) - \sum_n \sin^2(n\phi)|B_n|^2. \quad (18)$$

Equation (18) can be written more compactly by defining an inner product

$$\langle x|y\rangle = x^+S^+Sy \quad (19)$$

so Eq. (18) becomes

$$\langle \mathbf{u}|\mathbf{u}\rangle = \langle 1|1\rangle - \langle B|B\rangle. \quad (20)$$

As an aside, we mention that we could define

$$\mathbf{a}_r = S\mathbf{u}, \quad \mathbf{b}_l = S\mathbf{B} \text{ and } \mathbf{a}_l = S\mathbf{1} \quad (21)$$

so that Eq. (20) then reduces to Eq. (2) with $\mathbf{b}_r = \mathbf{0}$. Consequently the matrix $Q^{-1}RQ$ does act as a transfer matrix T satisfying Eqs. (3) and (5).

If we write P in terms of $N \times N$ matrices as

$$P = \begin{pmatrix} P_1 & P_2 \\ P_3 & P_4 \end{pmatrix} \quad (22)$$

then the relationships (14) can be solved to give

$$\mathbf{u} = (P_1 - P_2P_4^{-1}P_3)1 = p1, \quad (23)$$

$$\mathbf{B} = -P_4^{-1}P_3 1 = q1, \quad (24)$$

where p and q are the new transmission and reflection matrices [analogous to Eqs. (6) and (7)], and with

$$\mathbf{u}^+\mathbf{u} + \mathbf{B}^+\mathbf{B} = 1^+1 = N. \quad (25)$$

The transmission and reflection coefficients are now given by

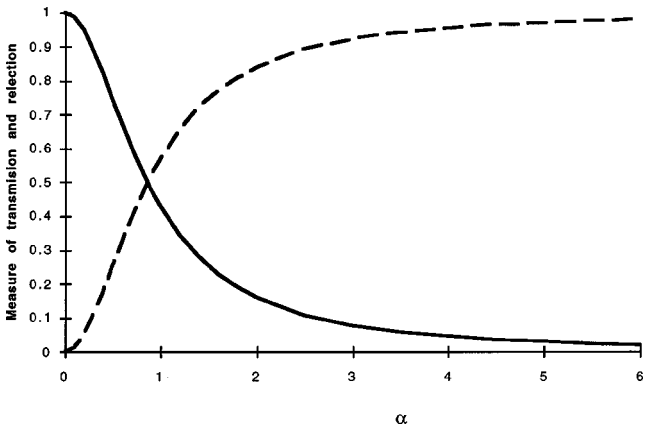

FIG. 2. The transmission (solid line) and reflection (dashed line) for the lattice of identical atoms as the tight-binding parameter α varies.

$$\tau = \frac{1^+ p^+ p 1}{1^+ 1} = \frac{\mathbf{u}^+ \mathbf{u}}{N}, \tag{26}$$

$$\rho = \frac{1^+ q^+ q 1}{1^+ 1} = \frac{\mathbf{B}^+ \mathbf{B}}{N}. \tag{27}$$

From Eq. (15) it can be seen that

$$P_i = S^{-1} T_i S, \quad i = 1,2,3,4, \tag{28}$$

where again the P_i's do not satisfy the relations (3) and (5). The analogous relationships that are satisfied by the P_i's can be found by substituting Eq. (28) into Eqs. (3) and (5), to obtain equations such as

$$p_1^+ S^2 P_1 - P_3^+ S^2 P_3 = S^2,$$

$$P_2^+ S^2 P_1 - P_4^+ S^2 P_3 = 0, \tag{29}$$

etc. Using Eq. (28) in Eq. (23), it is easy to show that the analog of Eq. (11) is

$$p = (P_1^*)^{-1} \tag{30}$$

(provided T_1 is symmetric). It can be noted that Eq. (30) is typically more convenient for calculations than is Eq. (23).

IV. ILLUSTRATIVE EXAMPLES AND CONCLUSIONS

Numerical examples. We illustrate the methodology with a couple of simple examples. First we look at the case of a periodic lattice of identical atoms. The tight-binding parameter α is varied while β is kept equal to 1. (For a detailed analysis of the tight-binding model used, see the Appendix.) The size of the lattice is determined by taking $N=6$ and $M=10$. We choose $\phi=\pi/7$ and within the leads we take $\alpha_1=0$ and $\beta_1=1$ and choose the periodicity so that $\theta=6\pi/7$. Then the energy of the particle is $E=0$. Figure 2 shows the variation of τ and ρ with α. When $\alpha=0$ (to match the energy E), perfect transmission is observed, as it should since $A_l - B - A_r$ is now an homogeneous material. As $|\alpha|$ increases, the transmission drops off quite rapidly, as E is no longer aligned with the band center, but is still within the band. When $|\alpha|=4$, E is aligned with a band edge and τ has largely vanished ($\tau = \approx 0.045$). As $|\alpha|$ increases further, τ drops off to 0.

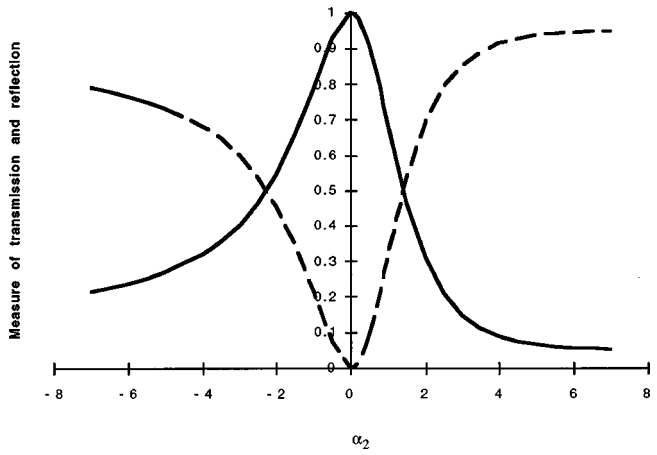

FIG. 3. The transmission (solid line) and reflection (dashed line) for a periodic lattice as the tight-binding parameter on one type of site α_2 varies and the equivalent parameter on the other sites is fixed so that $\alpha_1=0$.

As a second example, we take the lattice to be periodic, but with different atoms on adjacent sites, so that α alternates between α_1 and α_2. We take $\alpha_1=0$ and vary α_2 while taking all other parameters to have their values of Fig. 2. The variation of τ and ρ with α_2 is shown in Fig. 3, keeping $\alpha_1=0$. The results are mostly similar to those of Fig. 2 with perfect transmission when $\alpha_2=\alpha_1=0$, and then τ decreases as $|\alpha_2|$ increases. The graph is asymmetric about $\alpha_2=0$ because the band structure is not symmetric about the point $E=0$.

Aperiodic systems. We now discuss how the theory can be applied to aperiodic lattices. It is straightforward to apply the theory of the last section to a Fibonnacci lattice (or any similar rectangular lattice) where the sites are occupied by atoms *a* and *b* according to a deterministic but aperiodic prescription but it is much more difficult to treat nonrectangular lattices such as the Penrose tiling.

For the Penrose tiling the construction of the lattice is complex and we discuss how a rectangular lattice can be obtained using the technique of renormalization.[11] We first give a small example in detail to illustrate the method and then examine a larger example more briefly. A small section of a Penrose tiling is shown in Fig. 4(a) and we follow the convention of Ueda *et al.*[4] where the site of the atom is at the center of the rhombi. Atoms (11) and (12) interact with atoms (01) and (02), respectively, in region A_l and atoms (31) and (32) interact with (41) and (42), respectively, in A_r. We have two different rhombi (''fat'' rhombi and ''thin'' rhombi), representing the two types of atom in region *B*, but the arrangement is not rectangular. However, the theory of renormalization can be used to construct a rectangle. To illustrate this we note that the standard tight-binding model equations for this system are

$$(\alpha_1 - E)c_{11} + \beta(c_{12} + c_{21}) + \beta_0 c_{01} = 0, \tag{31a}$$

$$(\alpha_1 - E)c_{12} + \beta(c_{11} + c_{21}) + \beta_0 c_{02} = 0, \tag{31b}$$

$$(\alpha_2 - E)c_{21} + \beta(c_{12} + c_{21} + c_{31} + c_{32}) = 0, \tag{31c}$$

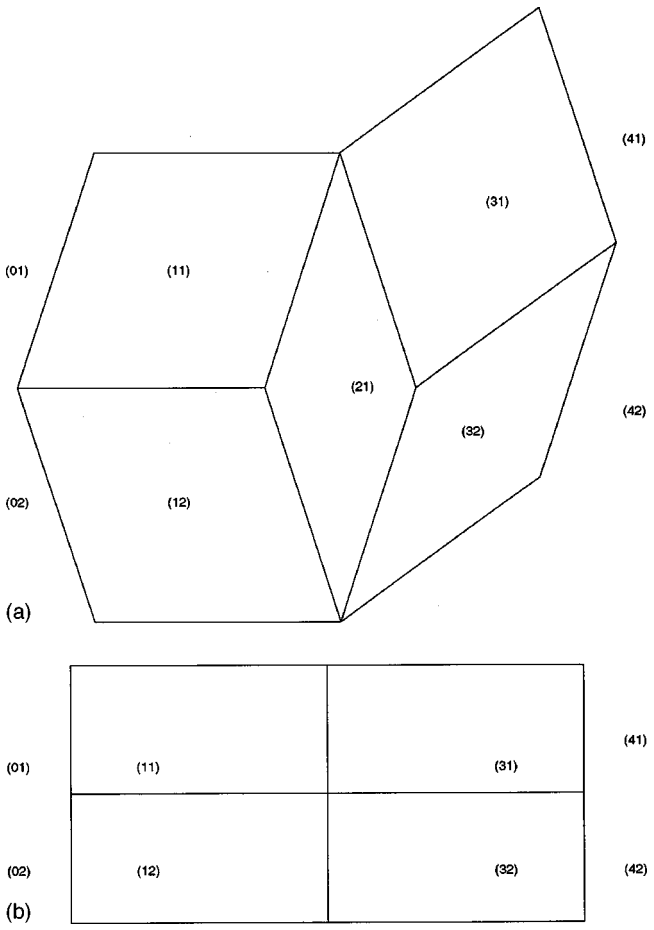

FIG. 4. (a) A small section of fat and thin rhombi, arranged in a Penrose tiling, with atoms at the centres of the rhombi. (b) A rectangular lattice, formed from Fig. 5(a) after renormalization; the atoms are at the centers of the rectangles.

$$(\alpha_1 - E)c_{31} + \beta(c_{32} + c_{21}) + \beta_0 c_{41} = 0, \tag{31d}$$

$$(\alpha_2 - E)c_{32} + \beta(c_{31} + c_{21}) + \beta_0 c_{42} = 0. \tag{31e}$$

Here the atoms at the center of the rhombi are numbered as in Fig. 4(a) and the values of α for the generally different atoms in the ''fat'' and ''thin'' rhombi are denoted by α_1 and α_2, respectively. The parameter β differs from β_0 since the latter is used for the interaction between region B and the other two outer regions.

These five equations can be reduced to four by the process of renormalization by eliminating c_{21} from Eq. (31c). We have

$$c_{21} = \frac{-\beta}{(\alpha_2 - E)}(c_{12} + c_{11} + c_{31} + c_{32}) \tag{32}$$

and we can substitute into the other equations so that for example (31a) becomes

$$\overline{\alpha} c_{11} + \beta_2 c_{12} + \beta_1(c_{31} + c_{32}) + \beta_0 c_{01} = 0, \tag{33}$$

where

$$\overline{\alpha} = (\alpha_1 - E) - \frac{\beta^2}{(\alpha_2 - E)}, \quad \beta_1 = -\frac{\beta^2}{(\alpha_2 - E)}$$

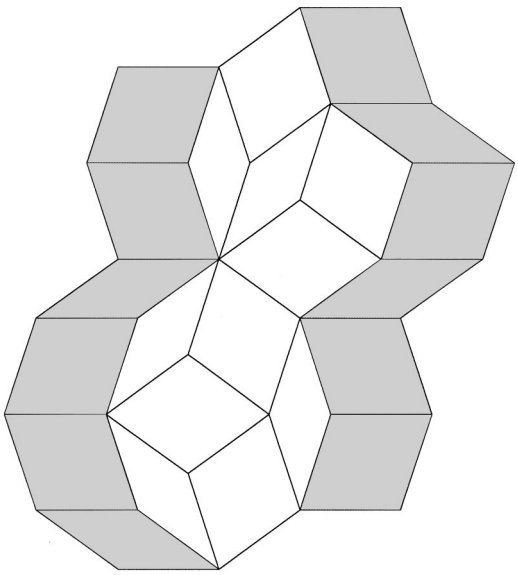

FIG. 5. A lattice arranged in a Penrose tiling with the atoms at the centers of the rhombi. The shaded rhombi on the edges denote those connected to leads.

$$\text{and} \quad \beta_2 = \beta - \beta_1 . \tag{34}$$

Similarly we can adjust the other equations in Eq. (31) and consequently we have a rectangular tight-binding system for which our theory may be applied [see Fig. 4(b)]. Note that the connections between the central region to the outer regions are unaltered in this scheme. If renormalization is carried out for these atoms the consequent interface conditions would be far more complicated.

We now illustrate a larger example of a piece of Penrose tiling in Fig. 5 where the darker shaded rhombi are those that are connected to leads. This too can be renormalized into a rectangular lattice, although we omit the algebraic details because they involve a set of 34 equations (for the 23 rhombi shown and the 12 leads). This can be renormalized so that the leads and the 12 connecting, dark shaded, rhombi on the left and right edges are renormalized to one rectangle apiece, while the center group of 11, light shaded, rhombi is renormalized to a column of 6 rectangles. The result of the renormalization is a 6×5 rectangular lattice (including the leads) to which the theory of the previous section can be applied.

CONCLUSIONS

In conclusion we have constructed a methodology to calculate transmission through a subsystem when the composite system is in a stationary state. We have confined our work to two-dimensional tight-binding lattices, and analyzed in detail the relationships between the submatrices of the ''transfer'' matrix. Applications to various systems will be the subject of future work.

ACKNOWLEDGMENTS

The work of K.W.S. has been supported by the Natural Sciences and Engineering Research Council of Canada.

APPENDIX

In this appendix we present the analysis of the tight-binding model used for each of the three materials considered and develop the mathematical analysis leading to Eqs. (12)–(17). In a tight-binding model we have discrete values of the amplitudes of the wave function and the corresponding Hamiltonian contains diagonal elements and interactions between neighboring atoms.

The wave function for the tight-binding model for the subsystems A_l and A_r is obtained by solving the equation

$$\alpha_1 c(m,n)+\beta_1[c(m,n+1)+c(m,n-1)+c(m+1,n)+c(m-1,n)] = Ec(m,n). \tag{A1}$$

This equation describes a two-dimensional rectangular lattice of identical atoms so that α_1, the diagonal terms in the Hamiltonian, are identical and the off-diagonal elements representing interactions with the four neighboring atoms are all β_1. This equation needs to be supplemented by boundary conditions and we choose the lattice so that it is periodic in the x direction and finite in the y direction. We also need to consider the conditions necessary to match these regions with the region B in which different assumptions are made in the tight-binding model. A solution of Eq. (A1) is

$$c(m,n)=e^{im\theta}e^{in\phi} \tag{A2}$$

for any real θ and ϕ and with

$$E=\alpha_1+2\beta_1\cos(\phi)+2\beta_1\cos(\theta). \tag{A3}$$

Other solutions with the same E can be obtained using $-\theta$ or $-\phi$ instead of θ and ϕ and the general solution is a linear combination of all possibilities. Here we consider region A_l to be $m\leqslant 0$, the region B to be $m=1\cdots M$, and the region A_r to be $m>M$ with $n=1\cdots N$ in all regions. The condition that the wave function is finite in the y direction is imposed to model a ''wire'' and, in region A_l, leads to a wave function in the form

$$c(m,n)=\sin(n\phi)(e^{im\theta}+B_n e^{-im\theta}), \quad m\leqslant 0, \tag{A4}$$

where

$$\sin[(N+1)\phi]=0 \tag{A5}$$

which implies that we may take $\phi=q\pi/(N+1)$, $q=1\cdots N$. The periodicity in the x direction for $m<1$ is imposed by choosing $\theta=2\pi v/M$, $v=0,\pm 1,\pm 2,\ldots$. A similar analysis can be made for the wave function in the region A_r but here, in our model, we impose an additional boundary condition to ensure that we only have outgoing waves in this subsystem. This leads to

$$c(m,n)=\sin(n\phi)D_n e^{im\theta}, \quad m>M. \tag{A6}$$

The constants B_n and D_n need to be chosen to match the wave function for the inner region, subsystem B. For this central subsystem B, the wave function coefficients are given by the standard tight-binding difference equation

$$(E-\alpha_{mn})c(m,n)=\beta[c(m+1,n)+c(m-1,n)+c(m,n+1)+c(m,n-1)] \tag{A7}$$

or

$$c(m+1,n)=-S_{mn}c(m,n)-c(m,n+1)-c(m,n-1)-c(m-1,n), \quad m=1\cdots M, \quad n=1\cdots N, \tag{A8}$$

where

$$S_{mn}=\frac{(\alpha_{mn}-E)}{\beta}. \tag{A9}$$

Equation (A8) can be rewritten in a more convenient vector form by defining

$$\psi(m)=[c(m,1),c(m,2)\cdots c(m,N)]^T. \tag{A10}$$

Then we can write

$$\begin{pmatrix}\psi(m+1)\\ \psi(m)\end{pmatrix}=R(m)\begin{pmatrix}\psi(m)\\ \psi(m-1)\end{pmatrix}, \tag{A11}$$

where $R(m)$ is the $(2N)\times(2N)$ matrix given by

$$R(m)=\begin{pmatrix}G(m) & -I\\ I & 0\end{pmatrix} \tag{A12}$$

and

$$G(m)=\begin{pmatrix}-S_{m1} & -1 & 0 & . & . & 0\\ -1 & -S_{m2} & -1 & 0 & . & 0\\ . & . & . & . & . & .\\ . & . & . & . & . & .\\ . & . & . & . & . & .\\ . & . & . & 0 & -1 & -S_{mN}\end{pmatrix}. \tag{A13}$$

Subsequently, we can connect the right and left edges of the lattice by writing

$$\begin{pmatrix}\psi(M+1)\\ \psi(M)\end{pmatrix}=\bar{\mathsf{R}}\begin{pmatrix}\psi(1)\\ \psi(0)\end{pmatrix}, \tag{A14}$$

where

$$\bar{\mathsf{R}}=R(M)R(M-1)\cdots R(2)R(1). \tag{A15}$$

We note that $R(1)$ and $R(M)$ could be modified to allow the β across the interface to differ from that in the lattice but for ease of presentation, we take them to be the same. Attaching subsystem B to A_l on the left is accomplished by taking

$$\begin{pmatrix}\psi(1)\\ \psi(0)\end{pmatrix}=R(0)\begin{pmatrix}\psi(0)\\ \psi(-1)\end{pmatrix}, \tag{A16}$$

where $R(0)$, through Eq. (A7), has some obvious replacements of α_{mn} and β by α_1 and β_1 when $m<1$. Similarly, attaching B to A_r is done by taking

$$\begin{pmatrix}\psi(M+2)\\ \psi(M+1)\end{pmatrix}=R(M+1)\begin{pmatrix}\psi(M+1)\\ \psi(M)\end{pmatrix}. \tag{A17}$$

Putting Eqs. (A16) and (A17) together with Eq. (A14) gives

$$\begin{pmatrix} \psi(M+2) \\ \psi(M+1) \end{pmatrix} = R \begin{pmatrix} \psi(0) \\ \psi(-1) \end{pmatrix}, \tag{A18}$$

where

$$R = R(M+1)\bar{\mathsf{R}}R(0). \tag{A19}$$

Note that the components of $\psi(M+2)$, $\psi(M+1)$, $\psi(0)$, and $\psi(-1)$ are the coefficients $c(m,n)$ with the forms given by Eqs. (12) and (13). Now we define

$$u_n = D_n e^{i(M+2)\theta} \tag{A20}$$

so from Eq. (13) we get

$$c(M+2,n) = \sin(n\phi)u_n, \quad c(M+1,n) = \sin(n\phi)u_n e^{-i\theta}. \tag{A21}$$

Equation (12) with $m = 0, -1$ gives

$$c(0,n) = \sin(n\phi)(1+B_n),$$

$$c(-1,n) = \sin(n\phi)(e^{-i\theta} + B_n e^{i\theta}). \tag{A22}$$

Thus Eq. (A18) can be written in matrix form as

$$QS_1 \begin{pmatrix} \mathbf{u} \\ \mathbf{0} \end{pmatrix} = RQS_1 \begin{pmatrix} \mathbf{1} \\ \mathbf{B} \end{pmatrix}, \tag{A23}$$

where $\mathbf{B} = (B_1, B_2, \ldots, B_N)^T$, etc.,

$$Q = \begin{pmatrix} I & I \\ Ie^{-i\theta} & Ie^{i\theta} \end{pmatrix}, \tag{A24}$$

$$S_1 = \begin{pmatrix} S & 0 \\ 0 & S \end{pmatrix}, \tag{A25}$$

and S is a diagonal matrix whose (n,n) element is $\sin(n\phi)$. Thus Eq. (A23) can be written as

$$\begin{pmatrix} \mathbf{u} \\ \mathbf{0} \end{pmatrix} = P \begin{pmatrix} \mathbf{1} \\ \mathbf{B} \end{pmatrix}, \tag{A26}$$

where

$$P = S_1^{-1} Q^{-1} R Q S_1. \tag{A27}$$

These relationships are then used in the analysis in Sec. III. One computational point should be mentioned. Suppose the real eigenvalues of the symmetric matrix $G(m)$ in Eq. (A13) are given by $g_i (i = 1 \cdots N)$. Then the eigenvalues of $R(m)$ in Eq. (A12) occur in pairs of the form

$$\lambda_i = \frac{g_i \pm \sqrt{g_i^2 - 4}}{2} \tag{A28}$$

showing that $R(m)$ is symplectic. If $|g_i| < 2$ for all i, then the λ_i are all complex with unit modulus. In this case the matrix multiplications of Eq. (A15) can be carried out without difficulty for any size of lattice. But if $|g_i| > 2$ for some i then the matrix elements of $\bar{\mathsf{R}}$ in Eq. (A15) increase rapidly in size with increasing M. The computation of Eqs. (A18) and (A19) is consequently more susceptable to numerical error and it is advisable to use very high precision. Here we used MAPLE, so that many of the computations can be done symbolically.

[1] H. Tsunetsugu and K. Ueda, Phys. Rev. B **38**, 10 109 (1988).
[2] H. Tsunetsugu, J. Phys. Soc. Jpn. **59**, 3057 (1990).
[3] H. Tsunetsugu and K. Ueda, Phys. Rev. B **43**, 8892 (1991).
[4] K. Ueda and H. Tsunetsugu, Phys. Rev. Lett. **58**, 1272 (1987).
[5] H. Schwabe, G. Kastner, and H. Bottger, Phys. Rev. B **56**, 8026 (1997).
[6] A. O. Barut and J. P. Dowling, Phys. Rev. Lett. **68**, 3571 (1992).
[7] D. Huang and G. Gumbs, Solid State Commun. **84**, 1061 (1992).
[8] M. Kolar and M. K. Ali, J. Phys.: Condens. Matter **1**, 823 (1989).
[9] Y. Imry, Europhys. Lett. **1**, 249 (1986).
[10] J. L. Pichard, Ph.D. thesis, University of Paris, Orsay, 1994.
[11] R. Farchioni, G. Grosso, and G. Parravicini, Phys. Rev. B **53**, 4294 (1996).