Eigenvalues and eigenfunctions of two coupled normal metal nano-rings

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Abstract
A general scheme is developed to deal with 1D lattice systems that could be topologically complicated. It is aimed to give a complete study of two coupled normal metal rings. Our method starts with an investigation of the local expressions of the eigenfunctions. By connecting different parts of the system, all the eigenvalues and eigenfunctions can be obtained. It is found that there is a possibility for the existence of localized states, which is beyond previous expectations.

Keywords: two coupled rings, transfer matrix, localized state

1. Introduction

The tight binding model is widely used to study electron behaviors in crystals. While it is originally suited for real materials that are of 3D, people are tempted to study the 1D case for simplicity. Usually only bulk properties are considered, so the Born-von Karman periodic boundary condition is chosen for convenience. The dispersion \( \epsilon = -2t \cos k \) is well-known for this 1D periodic tight-binding model [1]. Although open boundary conditions are most encountered in reality, it is generally believed that the physics in the bulk should not depend on any boundary conditions at least within the thermodynamic limit.

As technology develops, ever smaller systems are manufactured, and realistic 1D systems like quantum wires are realized. It happens that certain systems become sensitive to their boundary conditions due to small sizes. Additionally, the 1D models that theorists could only play with previously come to be relevant. In this background, some combined 1D systems were proposed, for example two coupled rings [2, 3]. To deal with models with complicated boundary conditions, a systematic method is in need.

In previous works on two coupled rings, two different methods were used. In [2], the method of Dirac constraints [4] was used. In [3], a simple wave function ansatz method was used. Since the focus of these papers was on persistent current [5–7], the solutions of the...
coupled system were studied only briefly and not in a complete way. Our present work is
dedicated to outline a general scheme to solve complicated 1D systems. By ‘solve’, we mean
to obtain all energy levels and corresponding eigenfunctions. In this paper the two coupled
rings problem is solved completely by this scheme.

Instead of the continuous model used in [2, 3], we choose to work with lattice models in
this work, because it has two advantages. First, the lattice model follows exactly the spirit of
tight binding, such that when the system becomes small to the extent of several nanometers,
the discreteness of atoms become important. Second, results can be checked easily by
diagonalizing Hamiltonian matrices numerically.

The usual way of doing quantum mechanics in 1D is to divide the system into several
homogeneous parts, obtain the general form of the wave function for each part first, and then
match them at the boundaries [8]. We will employ this standard procedure to study two
coupled rings. Before we jump into this complicated problem, however, it is pedagogical and
beneficial to start from simple situations that have simple boundary conditions. Thus we
would like to give a systematic review of 1D tight binding models, and see how different
boundary conditions could be treated.

We begin with a semi-infinite wire in section 2. Here the single open end of the wire is a
natural starting point for us to obtain eigenfunctions by iteratively applying Schrödinger
equations. We use a transfer matrix method to do the iterations. The general form of the
eigenfunction is determined by calculating the powers of the transfer matrix. Since there is
only one boundary condition for the semi-infinite wire, the eigenfunction can be easily
obtained.

In section 3 we study a finite open wire with two open ends. We employ the same scheme
by starting from one end and using the transfer matrix to obtain a general form of the
eigenfunction, while now the eigenfunction should also fulfil the boundary condition at the
other end. This gives us an additional equation that forms a constraint to the eigenvalues and
thus determines a discrete spectrum. In contrast, the semi-infinite wire has no such equation
and it has a continuous spectrum.

In section 4 a single closed ring is considered. The solution for this case is actually very
well known, since a Fourier transform can be applied to solve it almost immediately. While
now we do not turn to the Fourier transform method, we perform the same procedure as we do
for the finite open wire. This offers us an opportunity to test our scheme by comparing our
results to the familiar ones. An interesting point for the single closed ring is that we can thread
a magnetic flux through it, which leads to the Aharonov–Bohm effect [5] and persistent
currents [7]. For this situation, a gauge transform can be used to give the general result.

Section 5 is the focus of this paper, in which we study two coupled rings. Here we
assume the rings are connected by allowing electrons to hop between two selected sites. This
configuration is different from that considered in [2, 3], where there is a common site for both
rings. Actually our current scheme is capable to deal with both situations. But since our goal
is only to outline a general scheme and is not aimed to study all the possible models, we do
not study the common-site model in this work. To solve the problem first we get the local
form of the eigenfunction for each single ring. Then we use the boundary conditions to
connect the two local wave functions, and obtain an equation that determines all the eigen-
values. By studying this equation carefully, we find there can exist localized states. This
possibility is ignored in the previous works [2, 3].

We want to point out that the models and the results in sections 2–4 are not new but
actually well-known to experts. We present them here for the purpose to develop our scheme
to solve the two coupled rings in section 5. We hope it can also serve as a pedagogical reading
for non-experts. The results in section 5 are new and essential to this paper. The method we have employed can be generalized to deal with more complicated models.

2. Semi-infinite wire

We use the single band tight-binding model throughout this paper. It means on each lattice site there is one and only one state for a single electron. An electron can hop from one site to its nearest neighbours. Electrons are assumed spinless and non-interacting. The many particle states are composed by occupying single electron levels one by one.

Our starting point is a semi-infinite wire, of which the configuration is shown in figure 1. The most notable feature in this figure is that there is a single open end for the semi-infinite wire. The Hamiltonian under our assumption can be written in the formalism of second quantization as

\[ \hat{H} = -t \sum_{i=0}^{\infty} \hat{a}_i^\dagger \hat{a}_{i+1} + \text{h.c.}, \]  

(1)

where \( t \) is the hopping constant, \( \hat{a}_i^\dagger \) and \( \hat{a}_i \) are creation and annihilation operators for electrons on site \( i \).

Set \( \hat{\Lambda} = (\hat{a}_0, \hat{a}_1, \ldots )^T \), and rewrite the Hamiltonian in a matrix form

\[ \hat{H} = -t \hat{\Lambda}^\dagger \hat{\Lambda}, \]

(2)

where

\[ h = \begin{pmatrix} 0 & 1 & 1 & \cdots \\ 1 & 0 & 1 & \cdots \\ 1 & 0 & 1 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \]

(3)

is equivalent to the Hamiltonian matrix in the formalism of first quantization. Assume \( \psi = (x_0, x_1, \ldots )^T \) to be an eigenvector of \( h \) with eigenvalue \( \lambda \), then \( [x_0 \hat{a}_0^\dagger + x_1 \hat{a}_1^\dagger + x_2 \hat{a}_2^\dagger + \cdots ]|\Omega \rangle \) (\(|\Omega \rangle \) represents the vacuum state) is a single particle eigenstate of \( \hat{H} \) with energy level \( \epsilon = -\lambda t \). We would like to diagonalize \( h \), that is to say, we want to find all the eigenvalues of \( h \) and the corresponding eigenvectors. In this way we can obtain all the single particle eigenstates of \( \hat{H} \).

The eigenvalue equation of \( h \) reads

\[ \begin{pmatrix} 0 & 1 & 1 & \cdots \\ 1 & 0 & 1 & \cdots \\ 1 & 0 & 1 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} x_0 \\ x_1 \\ x_2 \\ \vdots \end{pmatrix} = \lambda \begin{pmatrix} x_0 \\ x_1 \\ x_2 \\ \vdots \end{pmatrix}. \]

(4)

It is also the time independent Schrödinger equation in the formalism of first quantization. Write equation (4) explicitly
\[
x_1 = \lambda x_0, \\
x_0 + x_2 = \lambda x_1, \\
x_1 + x_3 = \lambda x_2, \\
x_2 + x_4 = \lambda x_3, \\
\ldots \ldots
\]

Now if we set \( x_0 = 1 \), then \( x_1 = \lambda \). For \( n > 1 \), \( x_n = \lambda x_{n-1} - x_{n-2} \). By combining an obvious identity \( x_{n-1} = x_{n-1} \), we have

\[
\begin{pmatrix} x_n \\ x_{n-1} \end{pmatrix} = L \begin{pmatrix} x_{n-1} \\ x_{n-2} \end{pmatrix},
\]

where

\[
L = \begin{pmatrix} \lambda - 1 & 1 \\ 0 & 1 \end{pmatrix}
\]

is the so-called transfer matrix.

\( L \) is a constant matrix, independent of \( n \). We can iterate equation (5) and express \( (x_n, x_{n-1})^T \) in terms of \( (x_1, x_0)^T \) as

\[
\begin{pmatrix} x_n \\ x_{n-1} \end{pmatrix} = L^n \begin{pmatrix} x_1 \\ x_0 \end{pmatrix}.
\]

Now if we know \( L^n \) we can obtain the entire wave function. The calculation of \( L^n \) depends on the value of \( \lambda \). We summarize the results here and put its derivation in the appendix.

(i) If \( \lambda \in (-2, 2) \), set \( \lambda = 2 \cos \theta \), where \( \theta \in (0, \pi) \), then

\[
L^n = \begin{pmatrix} \sin(n+1)\theta & -\sin n\theta \\ \sin \theta & \sin \theta \\ \\
\sin n\theta & -\sin(n-1)\theta \\ \sin \theta & \sin \theta \end{pmatrix}.
\]  

(ii) If \( \lambda = 2 \), then

\[
L^n = \begin{pmatrix} n+1 & -n \\ n & -(n-1) \end{pmatrix}
\]

which corresponds to \( \theta \to 0 \) in (8).

If \( \lambda = -2 \), then

\[
L^n = (-1)^n \begin{pmatrix} n+1 & -n \\ n & -(n-1) \end{pmatrix}
\]

which corresponds to \( \theta \to \pi \) in (8).

(iii) If \( \lambda > 2 \), set \( \lambda = 2 \cosh k \), where \( k > 0 \), then

\[
L^n = \begin{pmatrix} \sinh(n+1)k & -\sinh nk \\ \sinh k & \sinh k \\ \\
\sinh nk & -\sinh(n-1)k \\ \sinh k & \sinh k \end{pmatrix}
\]

which corresponds to (8) if we set \( \theta = ik \).

If \( \lambda < -2 \), set \( \lambda = -2 \cosh k \), where \( k > 0 \), then
\[
L^n = (-1)^n \left( \frac{\sinh(n+1)k}{\sinh k} - \frac{\sinh nk}{\sinh k} \right) \tag{12}
\]

which corresponds to (8) if we set \( \theta = \pi + ik \).

Once we know \( L^n \), we can plug \( L^n \) into (7) and use the initial value \((x_0, x_1) = (1, \lambda)\) to write down the eigenfunction for each case:

(i) If \( \lambda = 2 \cos \theta \in (-2, 2), \theta \in (0, \pi) \)
\[
\psi = \left( 1, 2 \cos \theta, \frac{\sin 3\theta}{\sin \theta}, \frac{\sin 4\theta}{\sin \theta}, \ldots \right)^T. \tag{13}
\]

Note that \( U_n(\cos \theta) \equiv \frac{\sin(\alpha + 1)\theta}{\sin \theta} \) is the second kind of Chebyshev polynomial [9].

(ii) If \( \lambda = 2 \),
\[
\psi = (1, 2, 3, 4, \ldots)^T. \tag{14}
\]

If \( \lambda = -2 \),
\[
\psi = (1, -2, 3, -4, \ldots)^T. \tag{15}
\]

(iii) If \( \lambda > 2, \lambda = 2 \cosh k, k > 0 \)
\[
\psi = \left( 1, 2 \cosh k, \frac{\sinh 3k}{\sinh k}, \frac{\sinh 4k}{\sinh k}, \ldots \right)^T \tag{16}
\]

If \( \lambda < -2, \lambda = -2 \cosh k, k > 0 \)
\[
\psi = \left( 1, -2 \cosh k, \frac{\sinh 3k}{\sinh k}, \frac{\sinh 4k}{\sinh k}, \ldots \right)^T. \tag{17}
\]

In quantum mechanics wave functions are required to be normalizable, so they cannot blow up at infinity. Solutions (ii) and (iii) therefore should be abandoned. Thus the spectrum for a semi-infinite wire can only be in the range of \((-2, 2)\). Since we have no other constraint to the eigenvalue now, any value in \((-2, 2)\) belongs to the spectrum, so the spectrum of the semi-infinite wire is continuous.

In (i), if we set \( x_0 = \sin \theta \), the eigenfunction becomes
\[
\psi = (\sin \theta, \sin 2\theta, \sin 3\theta, \sin 4\theta, \ldots)^T. \tag{18}
\]

The form of this eigenfunction represents a standing wave with a single fixed end. It can be considered as the superposition of the incident wave and the reflected wave as the electron travels from infinity to the end and bounce back.

The wave function (18) cannot be normalized to 1 but can be normalized to a Dirac delta function. This happens due to the spectrum of the Hamiltonian is continuous. Since the spectrum is \((-2, 2)\) in the current case, the Hamiltonian operator is bounded. So the domain of the Hamiltonian operator is the whole Hilbert space [10, 11]. The Hamiltonian operator is also symmetric as shown in its matrix form (3), and thus it is self-adjoint [10, 11]. Any normalizable wave function can be expanded with respect to the basis (18).

We note here that in an early paper of Susskind and Glogower on the topic of quantum phase [12], the exactly same model of semi-infinite wire but in the guise of a different
physical situation was dealt with, through a slightly different method. Also, the half-line problem was studied in the mathematical literature like in [13].

Now we have finished the discussion of the semi-infinite wire. The key to the solution in this section is that we can express the entire wave function in terms of \((x_0, x_1)^T\) through (7). We note that the simple geometry of the semi-infinite wire gives us two great advantages. First, the single end of the wire supplies a natural starting point to begin the iterations. (Although in principle we can start from any two adjacent sites \((x_n, x_{n+1})^T\) and derive the entire wave function, it makes calculation more complicated.) Second, once we have obtained the general form of the eigenfunction, we need only further to consider the requirement of normalization, since there are no other boundary conditions.

In the following we vary the boundary conditions little by little, and see how our scheme can be adjusted readily for new situations.

3. Finite open wire

In this section we discuss the finite open wire, the configuration of which is shown in figure 2. Compared to the semi-infinite wire, it has two open ends and only a finite number of sites. Assume the number of sites is \(N\), and denote the wave function as \(\psi = (x_0, \ldots, x_N)^T\).

We would like to follow the same steps as before and start from the open end, since there is no difference in the local region of the end as compared to the semi-infinite wire. Let’s begin with \(x_1\) and \(x_2\) and use the transfer matrix to get the value of \(x_3, x_4, \ldots, x_N\). Now the difference from the semi-infinite wire is that we cannot go any further, because no site \((N + 1)\) exists. We have to stop here and require \(x_{N-1} = \lambda x_N\), which is the boundary condition at the other end of the wire.

It’s appropriate to use a little trick at this point. Imagine that we add site 0 at the left end and site \((N + 1)\) at the right end, and require that \(x_0 = x_{N+1} = 0\). Then the boundary conditions \(x_2 = \lambda x_1\) and \(x_{N-1} = \lambda x_N\) could be tailored as \(x_2 = \lambda x_1 - x_0\) and \(x_{N-1} = \lambda x_N - x_{N-2}\), which fits the general form of the iteration equation \(x_{n+1} = \lambda x_n - x_{n-1}\) for any \(n\). The advantage of this trick is that we have two much simpler boundary conditions \(x_0 = x_{N+1} = 0\) now.

We start from \(x_0(=0)\) and \(x_1\), use the transfer matrix and get a general expression of \(x_n\) for any \(n\). The form of \(x_n\) should be the same as that for the semi-infinite wire. Actually we can set \(x_1 = 1\), so \(x_2 = \lambda\), and then the same iterations as that of the semi-infinite wire follow.

After obtaining the expression \(x_n\) we need to require \(x_{N+1} = 0\). It’s obvious that there is no means for \(x_n\) to increase as \(n\) increases, so we have to abandon solutions (ii) and (iii). The eigenvalue \(\lambda\) stays in the range \((-2, 2)\) just like the case of the semi-infinite wire. For the semi-infinite wire any numbers in \((-2, 2)\) are possible spectrum, but now the additional equation \(x_{N+1} = 0\) is a constraint to \(\lambda\) and selects some specific values in \((-2, 2)\).

Set \(\lambda = 2\cos \theta\) \((0 < \theta < \pi)\), and \(x_0 = 0\), \(x_1 = \sin \theta\). Applying the transfer matrix (8), we have \(x_n = \sin n\theta\). From \(x_{N+1} = 0\), there is \(\sin(N + 1)\theta = 0\). This equation has \(N\) distinct roots.
They correspond to energy levels \( \epsilon_m = -\lambda_m t \) which constitute the complete spectrum. The eigenfunction with the energy level \( \epsilon_m \) is

\[
\psi_m \sim (0, \sin \theta_m, \sin 2\theta_m, \ldots, \sin N\theta_m, 0)^T,
\]

up to a normalization constant. It represents a standing wave that has two fixed ends.

Notice that the continuous version of our lattice model of the finite open wire is that of the particle in a box. From their solutions, the similarity is obvious.

In the mathematical literature, the corresponding problem of the finite open wire is dealt with in the theory of spectra of graphs \([14]\).

4. Single closed ring

If we connect the two ends of the finite open wire by allowing electrons to hop between the two end sites, then it forms a single closed ring. This configuration, as shown in figure 3, is equivalent to a 1D lattice with the Born-von Karman periodic boundary condition. Due to the translational symmetry, it is usually solved through Fourier transform. Now we want to develop our scheme to deal with the single closed ring and compare the results to the familiar ones.

Assume there are \( N \) sites on the ring, with the wave function \( \psi = (x_0, x_1, \ldots, x_{N-1})^T \). Just like what we have done in previous sections, we can start from \( x_0, x_1 \) and use the transfer matrix to attain \( x_n \) for arbitrary \( n \). Since now we have a periodic boundary condition, we expect that when \( n \) is larger than \( N \), \( x_n \) should be the same as \( x_{n-N} \). So we have \( x_N = x_0 \) and \( x_{N+1} = x_1 \). For

\[
\begin{pmatrix}
  x_{N+1} \\
  x_N
\end{pmatrix} = L^N
\begin{pmatrix}
  x_1 \\
  x_0
\end{pmatrix}
\]

thus

\[
\begin{pmatrix}
  x_1 \\
  x_0
\end{pmatrix} = L^N
\begin{pmatrix}
  x_1 \\
  x_0
\end{pmatrix}
\]
Before we move on, it is useful to unify all three different situations of $\lambda$ by enlarging the domain of $\theta$ in (i). As mentioned when we wrote down the expression of $L^n$ in section 2, we can extend the domain of $\theta$ into the complex plane, as shown in figure 4, to include all different situations. In the following we will use this generalized interpretation of $\theta$, and therefore $L^n$ could be simply expressed as (8).

Now insert (8) into (22) and we have

$$\begin{pmatrix} \frac{\sin(N+1)\theta}{\sin\theta} - 1 & -\frac{\sin N\theta}{\sin\theta} \\ -\frac{\sin N\theta}{\sin\theta} & \frac{\sin(N-1)\theta}{\sin\theta} - 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_0 \end{pmatrix} = 0. \tag{23}$$

If $x_0$ and $x_1$ are both zero, then $x_n = 0$ for any $n$. Thus, in order to get a non-zero eigenfunction, we have to first make sure (23) has a non-zero solution. So

$$\begin{pmatrix} \frac{\sin(N+1)\theta}{\sin\theta} - 1 & -\frac{\sin N\theta}{\sin\theta} \\ -\frac{\sin N\theta}{\sin\theta} & \frac{\sin(N-1)\theta}{\sin\theta} - 1 \end{pmatrix} = 0. \tag{24}$$

The roots of this equation represent the spectrum of the single closed ring. After fixing $\theta$, the ratio of $x_1$ and $x_0$ could be readily obtained through (23). The exact values of $x_1$ and $x_0$, up to a global phase, can be determined by normalization. The eigenfunction can be expressed in terms of $x_0$ and $x_1$ through (8) as

$$x_n = \frac{\sin n\theta}{\sin\theta} x_1 - \frac{\sin(n-1)\theta}{\sin\theta} x_0. \tag{25}$$

We do not give the detailed form of the eigenvalue and the eigenfunction for the single closed ring right now. We want to generalize the model by letting magnetic flux thread the ring. We will study this generalized model carefully. The solution of this generalized model will automatically include that of the ring with no magnetic flux as a special circumstance.

Let’s thread a magnetic flux $\Phi$ through the ring. (This makes the system a setup for the Aharonov–Bohm effect and the persistent current.) The well-known Peierls substitution can
be used to include the effect of the magnetic flux into the tight-binding model. Simply speaking, the Peierls substitution varies the hopping constant $t$ by a phase $\phi$, such that $t$ is substituted by $te^{i\phi}$. The phase $\phi$ is related to the vector potential $A$ via $\phi = (q/\hbar) \int_{i}^{i+1} A \cdot dr$. We can choose a gauge to let $A$ have the same magnitude along the ring, and so the result does not depend on the site number $i$ in the expression of $\phi$. Now $\Phi = \oint A \cdot dr$ is the total flux. If $\Phi = 0$, then $A = 0$ and thus $\phi = 0$.

After the introduction of magnetic flux, the Hamiltonian for the single closed ring can be written as

$$\hat{H} = -\sum_{i=0}^{N-1} te^{i\phi} \hat{a}_{i+1}^{\dagger} \hat{a}_i + \text{h.c.},$$

(26)

where $\hat{a}_N = \hat{a}_0$ is assumed for the ring’s topology.

We could turn this into a matrix form as (2) and would like to diagonalize the matrix $h_\phi$.

To emphasize the difference, we change the notation a little and set the eigenfunction of $h_\phi$ to be $(y_0, y_1, \ldots, y_{N-1})^T$.

Now the Schrödinger equation (the eigenvalue equation of $h_\phi$) becomes

$$y_{n-1}e^{-i\phi} + y_{n+1}e^{i\phi} = \lambda y_n,$$

(27)

where we set $\lambda = 2 \cos \theta$ under the generalized interpretation of $\theta$. This equation differs from our familiar one $x_{n-1} + x_{n+1} = \lambda x_n$ only by a gauge transform. If we set $y_n = e^{-i\phi} x_n$ then they are the same. Thus, based on the result (25), we have

$$y_n = \frac{\sin n\theta}{\sin \theta} e^{-i(n-1)\phi} y_{i-1} - \frac{\sin(n - 1)\theta}{\sin \theta} e^{-i\phi} y_0.$$  

(28)

Next, the boundary condition could be expressed similar to (22) as

$$y_0 = \frac{\sin N\theta}{\sin \theta} e^{-i(N-1)\phi} y_{i-1} - \frac{\sin(N - 1)\theta}{\sin \theta} e^{-i\phi} y_0,$$

(29)

$$y_1 = \frac{\sin(N + 1)\theta}{\sin \theta} e^{-iN\phi} y_{i-1} - \frac{\sin N\theta}{\sin \theta} e^{-i(N+1)\phi} y_0.$$  

(30)

Although (29) and (30) are of equal status now, they are not in the two coupled rings system that we will consider in the next section. Due to the coupling, (30) will be substituted by a different equation. However (29) will still hold. From (29) we can express $y_1$ in terms of $y_0$

$$y_1 = \frac{e^{i\phi} \sin \theta + e^{-i\phi} \sin(N - 1)\theta}{\sin N\theta} e^{i(N-1)\phi} y_0.$$  

(31)

Then plug (31) into (28), we have

$$y_n = \frac{e^{i(N-n)\phi} \sin n\theta + e^{-i\phi} \sin(N - n)\theta}{\sin N\theta} y_0.$$  

(32)

One notable property of this wave function is $y_{N-n} = y_n^*$, which means that the system remains the same if we reverse both the direction of the magnetic flux and the direction of the ring. The denominator $N\theta$ may equal to zero, but it occurs only accidentally, which results from a degeneracy that could be lifted by a small perturbation of the flux.

In (27) if we set $n = 0$ there is

$$y_{N-1}e^{-i\phi} + \gamma_1 e^{i\phi} = 2 \cos \theta y_0,$$

(33)

where the periodic boundary condition is used for the substitution of $y_{-1}$ to $y_{N-1}$. Combine (32) with (33), after simplification we get
The solution of (34) is shown in figure 5(a). Generally we have

\[ \theta = \frac{m}{N} 2\pi \pm \phi, \]  

where \( m \) belongs to the set of integers resulting in \( \theta \in [0, \pi] \). There are total \( N \) such integers, which thus constitute the complete spectrum.

Now if \( \phi \) varies, the spectrum \( \theta \) varies accordingly. But different \( \theta \)s vary in different directions as shown in figure 5(b), depending on whether they have ‘+’ or ‘−’ in (35).

We can enlarge the domain of \( \theta \) to \([-\pi, \pi]\) and reflect all the \( \theta \)s with ‘−’ sign to the interval \([-\pi, 0]\) as shown in figure 5(c)

\[ \frac{m}{N} 2\pi - \phi \rightarrow -\left(\frac{m}{N} 2\pi - \phi\right) = -\frac{m}{N} 2\pi + \phi. \]  

In this way we obtain a unified expression for \( \theta \)

\[ \theta = \frac{m}{N} 2\pi + \phi, \]  

where \( m \) belongs to the set of integers that let \( \theta \in [-\pi, \pi] \). Now as \( \phi \) varies, all the \( \theta \)s move in a consistent direction, as shown in figure 5(d).

Plug (37) in (32) and we have

\[ y_n = e^{im(\theta - \phi)} y_0. \]  

To normalize the eigenfunction, we can set \( y_0 = \frac{1}{\sqrt{N}} \).

Actually (37) and (38) can be easily obtained from a direct Fourier transform. So this justifies our scheme.

In the mathematical literature, the corresponding problem of the single closed ring is dealt with in the theory of spectra of graphs [14].
We have finished the discussion of the single closed ring now. It serves us a good preparation for the problem of two coupled rings.

5. Two coupled rings

The configuration of two coupled rings is shown in figure 6. We assume the rings have equal sizes and electrons are allowed to tunnel between the left ring site \( y_0 \) and the right ring site \( z_0 \). Magnetic flux \( \Phi_1 \) is threaded into the left ring and magnetic flux \( \Phi_2 \) is threaded into the right ring. The Hamiltonian could be cast into

\[
\hat{\mathcal{H}} = \hat{\mathcal{H}}_1 + \hat{\mathcal{H}}_2 + \hat{\mathcal{H}}_{\text{coupling}},
\]

where

\[
\hat{\mathcal{H}}_1 = - \sum_{i=0}^{N-1} [e^{i\Phi_1} \hat{a}_{i+1}^\dagger \hat{a}_i + \text{h.c.}],
\]

\[
\hat{\mathcal{H}}_2 = - \sum_{j=0}^{N-1} [e^{i\Phi_2} \hat{b}_{j+1}^\dagger \hat{b}_j + \text{h.c.}],
\]

\[
\hat{\mathcal{H}}_{\text{coupling}} = - V_0 (\hat{a}_0^\dagger \hat{b}_0 + \hat{b}_0^\dagger \hat{a}_0).
\]

\( \hat{\mathcal{H}}_1 \) and \( \hat{\mathcal{H}}_2 \) are two separate single closed ring Hamiltonians. \( \hat{\mathcal{H}}_1 \) is for the left ring, \( \hat{\mathcal{H}}_2 \) for the right ring. \( \hat{\mathcal{H}}_{\text{coupling}} \) represents the coupling between the two rings. In the expressions of \( \hat{\mathcal{H}}_1 \) and \( \hat{\mathcal{H}}_2 \) above, it is assumed \( \hat{a}_N = \hat{a}_0 \) and \( \hat{b}_N = \hat{b}_0 \) for the ring topology.

We emphasize here that the model in [2, 3] is different. In [2, 3], \( y_0 \) and \( z_0 \) are combined to a single site. This site then connects to \( y_1, y_{N-1}, z_1 \) and \( z_{N-1} \) separately.

Set the eigenfunction to be \( \psi = (y_1, y_2, \ldots, y_{N-1}, y_0, z_0, z_1, \ldots, z_{N-1})^T \). First, we can express the wave function on the left ring in terms of \( y_0 \) and the wave function on the right
ring in terms of \( z_0 \) separately, exactly the same as what we did for the single closed ring. So like (32), we could have

\[
y_0 = \frac{e^{i(N-n)\phi_1} \sin n\theta + e^{-im\phi_1} \sin (N-n)\theta}{\sin N\theta} y_0
\]

(43)

\[
z_0 = \frac{e^{i(N-n)\phi_2} \sin n\theta + e^{-im\phi_2} \sin (N-n)\theta}{\sin N\theta} z_0.
\]

(44)

Next, let us write down the Hamiltonian (39) in the matrix form

\[
\hat{H} = -\hat{A}^\dagger \hat{A}
\]

(45)

where \( \hat{A} = (\hat{a}_1, \hat{a}_2, \ldots, \hat{a}_{N-1}, \hat{a}_0, \hat{b}_0, \hat{b}_1, \ldots, \hat{b}_{N-1})^T \), and

\[
h = \begin{pmatrix}
0 & te^{i\phi_1} & \cdots & te^{-i\phi_1} \\
t e^{-i\phi_1} & \ddots & \ddots & \vdots \\
\vdots & \ddots & \ddots & te^{i\phi_1} \\
t e^{i\phi_1} & \cdots & te^{-i\phi_1} & 0
\end{pmatrix}
\]

(46)

\[
y_{N-1}te^{-i\phi_1} + y_1te^{i\phi_1} + V_0z_0 = \lambda y_0
\]

(47)

\[
z_{N-1}te^{-i\phi_2} + z_1te^{i\phi_2} + V_0y_0 = \lambda z_0.
\]

(48)

where \( \lambda \) is the eigenvalue of \( h \) (the single level energy is \( \epsilon = -\lambda \) under our notation). Set \( \lambda = 2t \cos \theta \) under the generalized interpretation of \( \theta \). Plug (43) and (44) into (47) and (48) to get

\[
\begin{pmatrix}
2t \sin \theta (\cos N\theta - \cos N\phi_1) & -V_0 \sin N\theta \\
-V_0 \sin N\theta & 2t \sin \theta (\cos N\theta - \cos N\phi_2)
\end{pmatrix}
\begin{pmatrix}
y_0 \\
z_0
\end{pmatrix} = 0.
\]

(49)

In order to get a non-zero solution, we have

\[
\begin{pmatrix}
2t \sin \theta (\cos N\theta - \cos N\phi_1) & -V_0 \sin N\theta \\
-V_0 \sin N\theta & 2t \sin \theta (\cos N\theta - \cos N\phi_2)
\end{pmatrix}
\begin{pmatrix}
y_0 \\
z_0
\end{pmatrix} = 0.
\]

(50)

So

\[
\frac{V_0^2 \sin^2 N\theta}{4t^2 \sin^2 \theta} = (\cos N\theta - \cos N\phi_1)(\cos N\theta - \cos N\phi_2).
\]

(51)

Equation (51) is the main result of this paper. The solution of (51) determines the spectrum of the two coupled rings system.

It is noted that \( N\phi_1 \) is proportional to the total flux that threads into the left ring. Actually \( N\phi_1 = \frac{\Phi_0}{\Phi_0} \pi \), where \( \Phi_0 \) is the flux quantum. \( N\phi_1 \) is the total phase that an electron could acquire due to magnetic flux \( \Phi_1 \) as it goes around one circle along the left ring. If this phase equals to \( 2\pi \), there should be no observable effect. Now since the only term involving \( \phi_1 \) in
is \( f_{N1} \cos \theta \), it is obvious that if we substitute \( f_{N1} \) by \( f_{p1} + N2 \), equation (51) remains the same. Likewise for \( f_{N2} \) and the right ring.

The two rings are coupled through the term \( \hat{H}_{\text{coupling}} \). If there is no coupling, or to say \( V_0 = 0 \) (so \( \hat{H}_{\text{coupling}} = 0 \)), then we expect to have two separate rings. Now through (51) it is clear that if \( V_0 = 0 \), we have \( \cos N\theta - \cos N\phi_1 = 0 \) or \( \cos N\theta - \cos N\phi_2 = 0 \). It means the rings decouple and the electron could only move on one of them.

At this level, we do not try to make a complete analysis of the equation (51). It should be very complicated since (51) is a transcendental equation. Instead, we want to use an example to show how the solutions of (51) look like.

Let \( N = 8, V_0 = t = 1 \) and choose two random fluxes \( \phi_1 \) and \( \phi_2 \). Figure 7 shows a sketch on how the solutions of (51) look with these parameters.

In figure 7(a), we show the situation when \( \lambda \) is in the range \([-2, 2]\) (\( \theta \) is real and in the range \([0, \pi]\)). The states here are propagating ones, for which the electron could move freely on both rings. As we will see, the wave functions of these states represent charge density waves. It may seem that all the eigenstates should belong to this kind, but that is not the case. There are 16 sites in our setup, so we should expect 16 eigenstates in total. We could find 14 intersections in figure 7(a), which correspond to only 14 eigenvalues and eigenstates. Thus there must exist two eigenstates that are not propagating states, of which the eigenvalues are beyond the interval \([-2, 2]\).

If \( \lambda > 2 \), we could use the general interpretation of \( \theta \) and set it to be \( ik \). Figure 7(b) shows there is a root in this range. So there is an eigenvalue in the range \((2, \infty)\). Similarly, there exists an eigenvalue in the range \((-\infty, -2)\), although we do not show it explicitly here.

The eigenstates of which the eigenvalues are not in \([-2, 2]\) correspond to localized states (bound states). As we will see, in this situation the wave function is localized around the junction and decays exponentially as it goes away from the junction. We have never met such kind of localized states before. It appears neither on the semi-infinite wire, nor on the finite wire, nor on the single closed ring. Also, we note that the possibility of the existence of the localized states has never been mentioned in the previous works on two coupled rings.

Next we want to discuss the local density of states and the normalization of the wave functions. Now assume \( \theta \) is a solution of (51). From (43) and (44), we have

**Figure 7.** Solutions of (51), the equation that determine the complete spectrum of the two coupled rings. Note: we set \( N = 8, V_0 = t = 1 \) in this plot. (a) the situation when the eigenvalue \( \lambda \) is in the range \([-2, 2]\) and we set \( \lambda = 2 \cos \theta \); (b) the situation when the eigenvalue \( \lambda \) is in the range \([2, \infty)\) and we set \( \lambda = 2 \cosh k \).
From (49), there is

\[
\frac{|\gamma_0|^2}{|\gamma_0|^2} = \frac{\sin^2 n\theta + \sin^2(N - n)\theta + 2\sin n\theta \sin(N - n)\theta \cos N\phi_1}{\sin^2 N\theta}
\]

Equations (52)–(54) show the relative magnitude of the eigenstate's local density. When \( \theta \) is in the range \([0, \pi]\), it is obvious that the local density is oscillating on each ring. So it represents a charge density wave and we say that the state is a propagating one. When \( \theta \) is out of the range \([0, \pi]\), we could use \( k \) to substitute \( \theta \) either by \( \theta = ik \) (when \( \lambda > 2 \)) or by \( \theta = \pi + ik \) (when \( \lambda < -2 \)). Then \( \cos n\theta \) and \( \sin n\theta \) could be substituted by \( \pm \cosh nk \) and \( \pm \sinh nk \). Since \( \cosh nk \) and \( \sinh nk \) are basically proportional to \( e^{\lambda n} \), it is easy to see that the local density is largest at the junction region, and decays exponentially away from it. In this sense, we have a localized state.

We can use the trigonometric identities

\[
\sum_{n=0}^{N-1} \frac{\sin^2 n\theta}{N} = \frac{N}{2} - \frac{\sin N\theta \cos(N - 1)\theta}{2\sin \theta}
\]

\[
\sum_{n=0}^{N-1} \frac{\sin^2(N - n)\theta}{N} = \frac{N}{2} - \frac{\sin N\theta \cos(N + 1)\theta}{2\sin \theta}
\]

\[
\sum_{n=0}^{N-1} 2\sin n\theta \sin(N - n)\theta = \cot \theta \sin N\theta - N\cos N\theta
\]

to sum (52) and (53) for all sites \( n \)

\[
\sum_{n=0}^{N-1} \frac{|\gamma_0|^2}{|\gamma_0|^2} = N(1 - \cos N\theta \cos N\phi_1) + \cot \theta \sin N\theta (\cos N\phi_1 - \cos N\theta)
\]

\[
\sum_{n=0}^{N-1} \frac{|\zeta_0|^2}{|\zeta_0|^2} = N(1 - \cos N\theta \cos N\phi_2) + \cot \theta \sin N\theta (\cos N\phi_2 - \cos N\theta)
\]

We can combine (54)–(56) to normalize the wave function and obtain the values of \( |\gamma_0| \) and \( |\zeta_0| \). The exact values of \( \gamma_0 \) and \( \zeta_0 \) are determined by equation (49) and the normalization of the wave function. Since the final expression is very long and gives little insight, we do not write it explicitly here.

6. Conclusion

We have developed a general scheme to study 1D single band tight binding models with complicated boundary conditions. The two coupled rings problem has been analysed step by step in this framework. The eigenvalues and eigenfunctions are given in a complete way. Our scheme starts from an investigation of the local property of the wave function. We find that in a homogeneous region, an explicit form of the wave function can be readily obtained in terms of its values on two nearest neighbour sites by a transfer matrix method.
Then with the boundary conditions for some special sites expressed specifically, we are able to obtain an equation to determine the complete spectrum.

Note that we divide the range of the eigenvalue \( \lambda \) mainly into two different cases. One is in \([-2, 2]\), and the other is out of \([-2, 2]\). For the former, the corresponding eigenstates are propagating waves. For the latter, the eigenstates are localized, which represent bound states. We have found that in our model of two coupled rings, there could exist bound states, which are localized around the junction.

The potential applications of these localized states are unclear at this moment. We expect that if we couple many rings together and form a kind of nano-ring network, then at each junction there exists a localized state. The wave functions of the localized states at different junctions could have small overlaps, and so electrons are able to tunnel from one junction to a nearby junction. In this way, we obtain a new lattice, formed by junctions between nearby nano-rings. Obviously, the lattice constant and the hopping constant can be adjusted by changing the size of the nano-rings.

Finally, we would like to point out that the method we have used in this paper is not restricted to the single band model. It is also possible to be applied to multi-band tight binding models. In such circumstances, the transfer matrices are more complicated.

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**Appendix. The calculation of \( L^n \)**

In this appendix we derive the expression of \( L^n \), the result of which is shown in the main text from equations (8) to (12).

From (6) the transfer matrix \( L \) is

\[
L = \begin{pmatrix} \lambda & -1 \\ 1 & 0 \end{pmatrix},
\]

where \( \lambda \) is a real number, corresponding to the eigenvalue of the original Hamiltonian \( h \).

Let us try to find the eigenvalue of \( L \) first. Assume \((a, b)^T\) is an eigenvector of \( L \) with eigenvalue \( \eta \). So

\[
\begin{pmatrix} \lambda & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \eta \begin{pmatrix} a \\ b \end{pmatrix}
\]

or

\[
\begin{pmatrix} \lambda - \eta & -1 \\ 1 & -\eta \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = 0.
\]
In order to get a non-zero eigenvector, we have to require

$$\begin{vmatrix} \lambda - \eta & 1 \\ 1 & \eta \end{vmatrix} = 0$$  \hspace{1cm} (A.4)$$

or

$$(\lambda - \eta)(-\eta) + 1 = 0.$$  \hspace{1cm} (A.5)$$

Thus

$$\eta = \frac{\lambda \pm \sqrt{\lambda^2 - 4}}{2}.$$  \hspace{1cm} (A.6)$$

Now according to the value of $\lambda$, it is necessary to separate the discussion into three different situations

(i) If $-2 < \lambda < 2$.

In this case we can set $\lambda = 2 \cos \theta$, where $0 < \theta < \pi$. And so

$$\eta_{1,2} = \frac{\lambda \pm \sqrt{\lambda^2 - 4}}{2} = \pm \frac{e^{i\theta}}{2}.$$  \hspace{1cm} (A.7)$$

For $\eta_1 = e^{i\theta}$, from (A.2) the corresponding eigenvector is

$$\begin{pmatrix} a_1 \\ b_1 \end{pmatrix} = \begin{pmatrix} e^{i\theta} \\ 1 \end{pmatrix}.$$  \hspace{1cm} (A.8)$$

For $\eta_2 = e^{-i\theta}$, from (A.2) the corresponding eigenvector is

$$\begin{pmatrix} a_2 \\ b_2 \end{pmatrix} = \begin{pmatrix} 1 \\ e^{i\theta} \end{pmatrix}.$$  \hspace{1cm} (A.9)$$

Now we can do a linear transform to diagonalize $L$. The transformation matrix is formed as

$$A = \begin{pmatrix} a_1 & a_2 \\ b_1 & b_2 \end{pmatrix} = \begin{pmatrix} e^{i\theta} & 1 \\ 1 & e^{i\theta} \end{pmatrix}.$$  \hspace{1cm} (A.10)$$

and $L$ can be written in the form

$$L = ADA^{-1} = A \begin{pmatrix} \eta_1 \\ \eta_2 \end{pmatrix} A^{-1},$$  \hspace{1cm} (A.11)$$

where

$$D = \begin{pmatrix} \eta_1 \\ \eta_2 \end{pmatrix} = \begin{pmatrix} e^{i\theta} \\ e^{-i\theta} \end{pmatrix}.$$  \hspace{1cm} (A.12)$$

and

$$A^{-1} = \frac{1}{\det(A)} \begin{pmatrix} b_2 & -a_2 \\ -b_1 & a_1 \end{pmatrix} = \frac{1}{e^{2i\theta} - 1} \begin{pmatrix} e^{i\theta} - 1 & -1 \\ -1 & e^{-i\theta} \end{pmatrix}.$$  \hspace{1cm} (A.13)$$

is the inverse of $A$.

Now $L^n$ can be calculated easily

$$L^n = \underbrace{(ADA^{-1})(ADA^{-1}) \cdots (ADA^{-1})}_{n} = AD^n A^{-1}.$$  \hspace{1cm} (A.14)$$

Since
\[ D^n = \begin{pmatrix} \eta_1^n \\ \eta_2^n \end{pmatrix} = \begin{pmatrix} e^{i\theta} \\ -e^{-i\theta} \end{pmatrix}. \]  
(A.15)

We have
\[ L^n = \frac{1}{e^{2i\theta} - 1} \begin{pmatrix} e^{i\theta} & 1 \\ 1 & e^{i\theta} \end{pmatrix} \begin{pmatrix} e^{i\theta} \\ -1 \end{pmatrix} \begin{pmatrix} e^{i\theta} \\ -1 \end{pmatrix}. \]  
(A.16)

Do this matrix multiplication, and after simplification we obtain
\[ L^n = \begin{pmatrix} \frac{\sin(n+1)\theta}{\sin \theta} & \frac{-\sin n\theta}{\sin \theta} \\ \frac{\sin n\theta}{\sin \theta} & \frac{-\sin(n-1)\theta}{\sin \theta} \end{pmatrix}. \]  
(A.17)

ii) If \( \lambda = \pm 2 \).

We only discuss the situation of \( \lambda = 2 \) here. In this case
\[ \eta = \frac{\lambda + \sqrt{\lambda^2 - 4}}{2} = 1. \]  
(A.18)

There is only one eigenvalue. From (A.2) we have the corresponding eigenvector
\[ \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}. \]  
(A.19)

There is no second linearly independent eigenvector. Thus \( L \) cannot be diagonalized. As a compromise, we try to find a vector \( (c, d)^T \) that fulfils
\[ L \begin{pmatrix} c \\ d \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix} + \eta \begin{pmatrix} c \\ d \end{pmatrix}. \]  
(A.20)

or
\[ \begin{pmatrix} 2 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} c \\ d \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix} + \begin{pmatrix} c \\ d \end{pmatrix}. \]  
(A.21)

So
\[ \begin{pmatrix} c \\ d \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \]  
(A.22)

Now we form a transformation matrix
\[ A = \begin{pmatrix} a & c \\ b & d \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}. \]  
(A.23)

and write \( L \) in the form
\[ L = ADA^{-1} = A \begin{pmatrix} \eta & 1 \\ 0 & \eta \end{pmatrix} A^{-1}, \]  
(A.24)

where
\[ D = \begin{pmatrix} \eta & 1 \\ 0 & \eta \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}, \]  
(A.25)

and
\[ A^{-1} = \begin{pmatrix} 0 & 1 \\ 1 & -1 \end{pmatrix}. \]  
(A.26)
is the inverse of $A$. Similar to the case $-2 < \lambda < 2$, we have

$$L^n = AD^nA^{-1}. \quad (A.27)$$

Now

$$D^n = \begin{pmatrix} \eta & 1 \\ 0 & \eta \end{pmatrix}^n = \begin{pmatrix} \eta^n & m\eta^{n-1} \\ 0 & \eta^n \end{pmatrix} = \begin{pmatrix} 1 & n \\ 0 & 1 \end{pmatrix}. \quad (A.28)$$

So

$$L^n = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & n \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & -1 \end{pmatrix} = \begin{pmatrix} n + 1 & -n \\ n & -(n - 1) \end{pmatrix} \quad (A.29)$$

(iii) If $\lambda > 2$ or $\lambda < -2$.

We only discuss the situation of $\lambda > 2$ here. Set $\lambda = 2 \cosh k$, where $k > 0$. So

$$\eta_{1,2} = \frac{\lambda \pm \sqrt{\lambda^2 - 4}}{2} = e^\pm k. \quad (A.30)$$

For $\eta_1 = e^k$, from (A.2) the corresponding eigenvector is

$$\begin{pmatrix} a_1 \\ b_1 \end{pmatrix} = \begin{pmatrix} e^k \\ 1 \end{pmatrix}. \quad (A.31)$$

For $\eta_2 = e^{-k}$, from (A.2) the corresponding eigenvector is

$$\begin{pmatrix} a_2 \\ b_2 \end{pmatrix} = \begin{pmatrix} 1 \\ e^k \end{pmatrix}. \quad (A.32)$$

Now we use a liner transform to diagonalize $L$. Form the transformation matrix

$$A = \begin{pmatrix} a_1 & a_2 \\ b_1 & b_2 \end{pmatrix} = \begin{pmatrix} e^k & 1 \\ 1 & e^k \end{pmatrix} \quad (A.33)$$

and $L$ can be written in the form

$$L = ADA^{-1} = A \begin{pmatrix} \eta_1 \\ \eta_2 \end{pmatrix} A^{-1}. \quad (A.34)$$

where

$$D = \begin{pmatrix} \eta_1 \\ \eta_2 \end{pmatrix} = \begin{pmatrix} e^k \\ e^{-k} \end{pmatrix} \quad (A.35)$$

and

$$A^{-1} = \frac{1}{\det(A)} \begin{pmatrix} b_2 & -a_2 \\ -b_1 & a_1 \end{pmatrix} = \frac{1}{e^{2k} - 1} \begin{pmatrix} e^k & -1 \\ -1 & e^k \end{pmatrix} \quad (A.36)$$

is the inverse of $A$.

Then

$$L^n = AD^nA^{-1} \quad (A.37)$$

and we have
\[ D^n = \begin{pmatrix} \eta_1^n \\ \eta_2^n \end{pmatrix} = \begin{pmatrix} e^{nk} \\ e^{-nk} \end{pmatrix}. \quad (A.38) \]

So

\[ L^n = \frac{1}{e^{2k} - 1} \begin{pmatrix} e^k & 1 \\ 1 & e^{-k} \end{pmatrix} \left( \begin{pmatrix} e^{nk} \\ e^{-nk} \end{pmatrix} \begin{pmatrix} e^k - 1 \\ -1 & e^k \end{pmatrix} \right) \quad (A.39) \]

or

\[ L^n = \begin{pmatrix} \frac{\sinh(n+1)k}{\sinh k} & -\frac{\sinh nk}{\sinh k} \\ \frac{\sinh nk}{\sinh k} & \frac{\sinh(n-1)k}{\sinh k} \end{pmatrix}. \quad (A.40) \]

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