Multi-channel quantum dragons in rectangular nanotubes

By

Zhou Li

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By

Zhou Li

Approved:

Mark A. Novotny
(Major Professor)

Seong-Gon Kim
(Committee Member)

R.Torsten Clay
(Committee Member)

Hendrik F. Arnoldus
(Graduate Coordinator)

R. Gregory Dunaway
Professor and Dean
College of Arts & Sciences

Name: Zhou Li

Date of Degree: May 9, 2015

Institution: Mississippi State University

Major Field: Physics

Major Professor: Dr. Mark A. Novotny

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Candidate for Degree of Master of Science

Recently the theoretical discovery of single channel quantum dragons has been reported. Quantum dragons are a class of nanodevices that may have strong disorder but still permit energy-independent total quantum transmission of electrons. This thesis illustrates that multi-channel quantum dragons also exit in rectangular nanotubes and provide an approach to construct multi-channel quantum dragons in rectangular nanotubes. Rectangular nanotube multi-channel quantum dragons have been validated by matrix method based quantum transmission calculation. This work could pave the way for constructing multi-channel quantum dragons from more complex nanostructures such as single-walled zigzag carbon nanotubes and single-walled armchair carbon nanotubes.

Key words: Electron transmission, Quantum dragons, Nanotubes,

DEDICATION

To my family and friends.

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TABLE OF CONTENTS

LIST OF FIGURES

CHAPTER 1

INTRODUCTION

1.1 Conductance from transmission

Electrical conductance G of an electrical conductor is defined as

$$G = \frac{I}{V} \tag{1.1}$$

where I is the current through the conductor and V is the voltage across the conductor. This proportionality is call Ohm's law.

When the dimensions of conductors become small enough, the classical ohmic behavior of the conductor breaks down. In such cases, quantum mechanics should be applied to study the properties such as conductance of the conductors. Landauer showed that the conductance G can be related to transmission probability as a function of energy, $\mathcal{T}(E)$, in the Landauer formula [14]

$$G = \frac{2e^2}{h}(\mathcal{I}_1 + \mathcal{I}_2 + \cdots) \,. \tag{1.2}$$

where each integral $\mathcal{I}_k$ contains the Fermi function and the transmission probability $\mathcal{T}_k$ of the kth channel for an impinging electron of energy E. Here e is the charge of an electron and h is Planck's constant. G_0 is the quantum of conductance $G_0 = 2e^2/h = 7.748^{-5} mhos$.

In a nanostructure with no disorder, electrons undergo ballistic propagation and hence have $\mathcal{T} = 1$[14]. Hence, for a ballistic conductor with M open channels at low temperatures

$$G = \frac{2e^2}{h} M \,. \tag{1.3}$$

Nanostructures with negligible scattering are ballistic. The effect of Anderson localization [2][9] showed that random disorder in 1D will localize the wave function and therefore make the transmission very small. This effect suggests that the transmission of any nanostructure with disorder will be non-ballistic and hence the conductance will be very small providing certain channels are opened. However in next section it will be shown that, presentation of correlated disorder will not localize the wavefunction and nanostructures with these kinds of disorder can also have electrons propagating with total transmission probability.

1.2 Definitions of quantum dragons

Recently, a class of nanostructures called quantum dragons have been reported[16]. Quantum dragons are nanodevices that may have disorder but the electron transmission probability in such structures is still unity for all propagating energies when connected to idealized leads. Therefore quantum dragons have zero electrical resistance in a four-probe measurement, and for a single open channel have G_0^{-1} electrical resistance in a two-probe measurement. This can be seen from the Landauer formula for a two-probe measurement and a four-probe measurement case [10], for a single channel at low temperatures,

$$G = \begin{cases} G_0\mathcal{T}(E_F) & \mathrm{two-probe} \\ \\ G_0\frac{\mathcal{T}(E_F)}{1-\mathcal{T}(E_F)} & \mathrm{four-probe} \end{cases} . \tag{1.4}$$

These expressions at low temperature come from Eq. (1.2), and for one open channel, the integral is

$$\mathcal{I} = \int \mathcal{T}(E)(\frac{\partial f}{\partial E})dE \approx \mathcal{T}(E_F) \,. \tag{1.5}$$

because the partial derivative of the Fermi function is approximately a delta function at the Fermi energy E_F.

The problem of how to find quantum dragons in nanodevices connected to 1D idealized leads has been studied in the original paper[16] in detail. To set the notation for the readers, the relavant equations are given in the Appendix.

1.3 Multi-channel quantum dragons

When a nanodevice is connected to idealized 1D leads, only one travelling wave mode can propagate through the structure, therefore only one energy channel is opened. In such cases, there will only be single channel quantum dragons. Single channel quantum dragons have conductance $G = G_0$. It is possible for non-1D idealized leads that permit more than one travelling wave mode, thus it is possible to have multi-channel quantum dragons in nanodevices that are connected to more complex idealized leads. For multi-channel quantum dragons, the conductance will be $G = G_0 M$, where M is the number of open channels.

This thesis studies multi-channel quantum dragons from rectangular nanotubes, trying to answer the key question what kind of rectangular nanostructures can be multi-channel quantum dragons. The general solution of the transmission is given first in Chapter 1, and two example multi-channel quantum dragons structures are shown in Chapter 2.

1.4 Methods to calculate the transmission

Quantum dragons are nanodevices when connected to idealized leads have full transmission of electrons for all energies. One needs to calculate the transmission of a nanodevice not only to find quantum dragons, but also to prove a nanodevice is indeed a quantum dragon.

Within the tight-binding approximation, three different methods are applied in the literature. There are the scattering theory technique[8], the Green's function method[8] and the matrix method[12][7][6]. Because of the ability of reducing the complexity of the problem in a large device, the matrix method was used to find quantum dragons in the original paper. The Appendix of this thesis shows how the reduction is done within the matrix method.

In the rest of this thesis, the matrix method framework is also used to study multi-channel quantum dragons. In Chapter 1 the matrix equation used to calculate the electron transmission of nanodevices is introduced. Examples of rectangular multi-channel dragons found within the matrix method framework are given in Chapter 2.

CHAPTER 2

MULTI-CHANNEL QUANTUM DRAGONS

2.1 Matrix equation for transmission calculation of nanodevice connected to non-1D leads

The question about how to find quantum dragon segments for blobs connected to single chain leads has been studied in [16]. An incoming lead and an outgoing lead are connected to a nanodevice when measuring the conductance G. The nanodevices that are connected to two leads are called the "blob". This chapter will focus on how to find quantum dragons segments for blobs connected to more complicated leads than a 1D chain. Also, the blob and lead throughout this thesis have linear forms, namely they are consisting of different slices and each slice only has interactions with its neighbor slices.

Consider the following diagram for a lead and blob configuration.

$$\begin{array}{ccccccccccccccccc} \cdots & \mathbf{B}_L & \rightarrow & (0) & \leftarrow & \mathbf{W} & \rightarrow & (a) & \leftarrow & \mathbf{B}_{ab} & \rightarrow & (b) & \leftarrow & \mathbf{U} & \rightarrow & (1) & \leftarrow & \mathbf{B}_L & \cdots \\ \cdots & & & \mathbf{A}_L & & & & \mathbf{A}_a & & & & \mathbf{A}_b & & & & \mathbf{A}_L & & & \cdots \\ \cdots & & & \vec{\Psi}_0 & & & & \vec{\Psi}_a & & & & \vec{\Psi}_b & & & & \vec{\Psi}_1 & & & \cdots \end{array} \tag{2.1}$$

where both blob slices a and b have been put between the $x = 0$ and $x = 1$ lead slices. $\mathbf{A}$ and $\mathbf{B}$ are intra and inter slice matrix connections, respectively. The subscript indicates which parts it describes. $\vec{\Psi}$ are block wavefunctions in different slices from the lead and the blob.

The semi-infinite incoming lead and its connection to the blob is shown in the following diagram

$$\begin{array}{ccccccccccccccc}
\cdots & (-3) & \leftarrow & \mathbf{B}_L & \rightarrow & (-2) & \leftarrow & \mathbf{B}_L & \rightarrow & (-1) & \leftarrow & \mathbf{B}_L & \rightarrow & (0) & \leftarrow & \mathbf{W} & \rightarrow & (a) & \cdots \\
\cdots & \mathbf{A}_L & & & & \mathbf{A}_L & & & & \mathbf{A}_L & & & & \mathbf{A}_L & & & & \mathbf{A}_a & \cdots \\
\cdots & \vec{\Psi}_{-3} & & & & \vec{\Psi}_{-2} & & & & \vec{\Psi}_{-1} & & & & \vec{\Psi}_0 & & & & \vec{\Psi}_a & \cdots
\end{array} \tag{2.2}$$

From this diagram, one has the infinite matrix equation $H\Psi = E\Psi$

$$\begin{pmatrix} \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \\ \cdots & \mathbf{A}_L & -\mathbf{B}_L & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \cdots \\ \cdots & -\mathbf{B}_L^T & \mathbf{A}_L & -\mathbf{B}_L & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \cdots \\ \cdots & \mathbf{0} & -\mathbf{B}_L^T & \mathbf{A}_L & -\mathbf{W} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \cdots \\ \cdots & \mathbf{0} & \mathbf{0} & -\mathbf{W}^T & \mathbf{A}_a & -\mathbf{B}_{ab} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \cdots \\ \cdots & \mathbf{0} & \mathbf{0} & \mathbf{0} & -\mathbf{B}_{ab}^T & \mathbf{A}_b & -\mathbf{U} & \mathbf{0} & \mathbf{0} & \cdots \\ \cdots & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & -\mathbf{U}^T & \mathbf{A}_L & -\mathbf{B}_L & \mathbf{0} & \cdots \\ \cdots & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & -\mathbf{B}_L^T & \mathbf{A}_L & -\mathbf{B}_L & \cdots \\ \cdots & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & -\mathbf{B}_L^T & \mathbf{A}_L & \cdots \\ & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} \vdots \\ \vec{\Psi}_{-2} \\ \vec{\Psi}_{-1} \\ \vec{\Psi}_0 \\ \vec{\Psi}_a \\ \vec{\Psi}_b \\ \vec{\Psi}_1 \\ \vec{\Psi}_2 \\ \vec{\Psi}_3 \\ \vdots \end{pmatrix} = E \begin{pmatrix} \vdots \\ \vec{\Psi}_{-2} \\ \vec{\Psi}_{-1} \\ \vec{\Psi}_0 \\ \vec{\Psi}_a \\ \vec{\Psi}_b \\ \vec{\Psi}_1 \\ \vec{\Psi}_2 \\ \vec{\Psi}_3 \\ \vdots \end{pmatrix} . \tag{2.3}$$

Without loss of generality, the leads consists of identical slices. If there are some slices in leads which are not the same with others, these parts can be included in the blob, leaving the remaining leads consisting of identical slices. The number of blob slices can be any integer number. In this diagram the blob consists of only two slices, for brevity of the equation.

From Eq. (2.3), the block wavefunctions from slices $-\infty, \cdots, -3, -2, -1$ and $2, 3, 4, \cdots, +\infty$ will be solved from

$$-\mathbf{B}_L^T \vec{\Psi}_{n-1} + (\mathbf{A}_L - E\mathbf{I})\vec{\Psi}_n - \mathbf{B}_L \vec{\Psi}_{n+1} = \vec{0}\,. \tag{2.4}$$

The slice wavefunctions from slices $0, a, b, 1$ will be solved from the remaining part of the matrix equation

$$\begin{pmatrix} -\mathbf{B}_L^T & \mathbf{A}_L - E\mathbf{I} & -\mathbf{W} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & -\mathbf{W}^T & \mathbf{A}_a - E\mathbf{I} & -\mathbf{B}_{ab} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & -\mathbf{B}_{ab}^T & \mathbf{A}_b - E\mathbf{I} & -\mathbf{U} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & -\mathbf{U}^T & \mathbf{A}_L - E\mathbf{I} & -\mathbf{B}_L \end{pmatrix} \begin{pmatrix} \vec{\Psi}_{-1} \\ \vec{\Psi}_0 \\ \vec{\Psi}_a \\ \vec{\Psi}_b \\ \vec{\Psi}_1 \\ \vec{\Psi}_2 \end{pmatrix} = \begin{pmatrix} \vec{0} \\ \vec{0} \\ \vec{0} \\ \vec{0} \end{pmatrix} \tag{2.5}$$

which is now a finite matrix equation.

Use Bloch's theorem to write the slice wavefunction for the leads as a travelling wave with wavevector q times the intra-slice wave function ϕ for both the incoming and outgoing leads.

In particular, the $ansatz$ for lead slice wavefunctions are

$$\begin{array}{ll} \vec{\Psi}_n = e^{iqn}\vec{\phi} + re^{-iqn}\vec{\phi}^* & n = -\infty, \cdots, -2, -1, 0 \\ \vec{\Psi}_n = t_T e^{iq(n-1)}\vec{\phi} & n = 1, 2, 3, \cdots, +\infty \end{array} . \tag{2.6}$$

The unit of length has been set to be the the distance between adjacent lead slices, and this length has been set to 1.

The $ansatz$ corresponds to a wave of unit intensity impinging on the blob from the left-hand (incoming) lead and being partially reflected back to $-\infty$ and partially transmitted to $+\infty$.

2.1.1 General solution of leads part of the matrix equation

In this subsection, the $ansatz$ is used to solve the block wavefunction for the leads. Let every slice of the leads have m_L atoms.

For $n = -\infty, \cdots, -2, -1, 0$ slices, substitute the first equation in Eq. (2.6) back into Eq. (2.5)

$$e^{iqn}[-\mathbf{B}_L^T e^{-iq}\vec{\phi} + (\mathbf{A}_L - E\mathbf{I})\vec{\phi} - \mathbf{B}_L e^{iq}\vec{\phi}] + re^{-iqn}[-\mathbf{B}_L^T \vec{\phi}^* + (\mathbf{A}_L - E\mathbf{I})\vec{\phi}^* - \mathbf{B}_L e^{-iq}\vec{\phi}^*] = \vec{0}. \tag{2.7}$$

For $n = 1, 2, 3, \cdots, +\infty$ slices, substitute the second equation in Eq. (2.6) back into Eq. (2.5)

$$e^{iq(n-1)} t_T [-\mathbf{B}_L^T e^{-iq}\vec{\phi} + (\mathbf{A}_L - E\mathbf{I})\vec{\phi} - \mathbf{B}_L e^{iq}\vec{\phi}] = \vec{0}\,. \tag{2.8}$$

Eq. (2.8) is satisfied provided

$$[-\mathbf{B}_L^T e^{-iq} + (\mathbf{A}_L - E\mathbf{I}) - \mathbf{B}_L e^{iq}]\vec{\phi} = \vec{0}\,. \tag{2.9}$$

Introduce the m_L eigenvectors ϕ_j and associated eigenvalues $\lambda_j(E,q)$ of the matrix $[-\mathbf{B}_L^T e^{-iq} + (\mathbf{A}_L - E\mathbf{I}) - \mathbf{B}_L e^{iq}]$. The eigen equation is

$$[-\mathbf{B}_L^T e^{-iq} + (\mathbf{A}_L - E\mathbf{I}) - \mathbf{B}_L e^{iq}]\vec{\phi}_j = \lambda_j(E,q)\vec{\phi}_j \; . \tag{2.10}$$

To find the wavevectors q in Eq. (2.10) , set

$$\lambda_j(E,q) = 0 \; . \tag{2.11}$$

Every eigenvalue will have its own wavevectors $q = q_j$.

Therefore, Eq. (2.9) is satisfied. Hence the $ansatz$ of Eq. (2.6) satisfies the Schrödinger equation for the outgoing lead of Eq.(2.8).

Provided equation Eq. (2.10) is satisfied, the first part of Eq. (2.7), which is the first square bracket, is $\vec{0}$. Therefore, the only equation to satisfy is the reflected part of Eq.(2.7).

Taking the complex conjugate of Eq.(2.10) gives

$$[-\mathbf{B}_L^{T*} e^{iq} + (\mathbf{A}_L^* - E\mathbf{I}) - \mathbf{B}_L^* e^{-iq}]\vec{\phi}_l^* = \lambda_j^*(E,q)\vec{\phi}_j^* \; . \tag{2.12}$$

We have assumed that $\mathbf{A}_L$ and $\mathbf{B}_L$ in all cases have only real components. Thus we have

$$[-\mathbf{B}_L^T e^{iq} + (\mathbf{A}_L - E\mathbf{I}) - \mathbf{B}_L e^{-iq}]\vec{\phi}_j^* = \lambda_j(E,q)\vec{\phi}_j^* \; . \tag{2.13}$$

$[-\mathbf{B}_L^T e^{-iq} + (\mathbf{A}_L - E\mathbf{I}) - \mathbf{B}_L e^{iq}]$ is Hermitian, so its eigenvalues are real, hence $\lambda_j^*(E,q) = \lambda_j(E,q)$. The left hand side of Eq. (2.13) is exactly the matrix component of the reflected part of Eq. (2.7). So q from Eq. (2.9) also satisfies Eq. (2.7). Thus the time-independent Schrödinger equation is satisfied for all lead slices except for slice 0 and slice 1 in the lead.

When sloving for wavevectors of the travelling waves, one can have m_L different $q = q_j(E)$, assuming that the lead matrix $\mathbf{A}_L$ and $\mathbf{B}_L$ are of dimensions $m_L \times m_L$. Wavevectors q should be real for travelling waves. So for each solution $q = q_j(E)$, namely different channels of propagating waves, each channel will have its own permitted energy range satisfying q being real.

2.1.2 Gernaral Solution of blob part of matrix equation

We have found the m_L wavevectors q_{m_L} that satisfied the lead part of the matrix Eq.(2.3). In this subsection, we use the $ansatz$ to simplify the blob part of the matrix equation.

Using the $ansatz$ for $n = -1, 0, 1, 2$ block wavefunctions, the Eq. (2.5) becomes

$$\begin{pmatrix} -\mathbf{B_L}^T & \mathbf{A_L} - E\mathbf{I} & -\mathbf{W} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & -\mathbf{W}^T & \mathbf{A}_a - E\mathbf{I} & -\mathbf{B}_{ab} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & -\mathbf{B}_{ab}^T & \mathbf{A}_b - E\mathbf{I} & -\mathbf{U} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & -\mathbf{U}^T & \mathbf{A}_L - E\mathbf{I} & -\mathbf{B}_L \end{pmatrix} \begin{pmatrix} e^{-iq_j}\vec{\phi}_j + r_j e^{iq_j}\vec{\phi}_j^* \\ \vec{\phi}_j + r_j\vec{\phi}_j^{\,*} \\ \vec{\psi}_a \\ \vec{\psi}_b \\ t_{Tj}\vec{\phi}_j \\ t_{Tj}e^{iq_j}\vec{\phi}_j \end{pmatrix} = \begin{pmatrix} \vec{0} \\ \vec{0} \\ \vec{0} \\ \vec{0} \end{pmatrix}. \tag{2.14}$$

Here $\vec{\phi}_j$ is one of the eigenvectors from the eigen equation (3.36), and the q_j is solved from setting the corresponding eigenvalue to 0: $\lambda_j(E, q_j) = 0$. The above equation is just a matrix equation for the channel j. Each channel will have different solutions for r_j and t_{Tj}. The transmission probability of channel j will be $\mathcal{T}_j(E) = |t_{Tj}(E)|^2$, and the reflection probability is $\mathcal{R}_j(E) = |r_j(E)|^2$. There are m_L such matrix equations in total.

Multiply through in Eq. (2.14)

$$\begin{pmatrix} (\mathbf{A}_L - E\mathbf{I} - e^{-iq_j}\mathbf{B_L}^T)\vec{\phi}_j + (\mathbf{A}_L - E\mathbf{I} - e^{iq_j}\mathbf{B_L}^T)r_j\vec{\phi}_j^{\,*} - \mathbf{W}\vec{\psi}_a \\ -\mathbf{W}^T(\vec{\phi}_j + r_j\vec{\psi}_j^*) + (\mathbf{A}_a - E\mathbf{I})\vec{\psi}_a - \mathbf{B}_{ab}\vec{\psi}_b \\ -\mathbf{B}_{ab}^T\vec{\psi}_a + (\mathbf{A}_b - E\mathbf{I})\vec{\psi}_b - \mathbf{U}t_{Tj}\vec{\phi}_j \\ -\mathbf{U}_T\vec{\psi}_b + t_{Tj}(\mathbf{A}_L - E\mathbf{I} - e^{iq_j}\mathbf{B}_L)\vec{\phi}_j \end{pmatrix} = \begin{pmatrix} \vec{0} \\ \vec{0} \\ \vec{0} \\ \vec{0} \end{pmatrix} . \quad (2.15)$$

The equation above can be written as a new matrix equation

$$\begin{pmatrix} \xi_{L,j} & -\mathbf{W} & \mathbf{0} & \mathbf{0} \\ -\mathbf{W}^T & \mathbf{A}_a - E\mathbf{I} & -\mathbf{B}_{ab} & \mathbf{0} \\ \mathbf{0} & -\mathbf{B}_{ab}^T & \mathbf{A}_b - E\mathbf{I} & -\mathbf{U} \\ \mathbf{0} & \mathbf{0} & -\mathbf{U}^T & \xi_{R,j} \end{pmatrix} \begin{pmatrix} \vec{\phi}_j + r_j\vec{\phi}_j^* \\ \vec{\psi}_a \\ \vec{\psi}_b \\ t_{Tj}\vec{\phi}_j \end{pmatrix} = \begin{pmatrix} -2i\sin(q_j)\mathbf{B}_L^T\vec{\phi}_j \\ \vec{0} \\ \vec{0} \\ \vec{0} \end{pmatrix} \quad (2.16)$$

with the definitions

$$\xi_{L.j} = \mathbf{A}_L - E\mathbf{I} - e^{iq_j}\mathbf{B}_L^T \quad (2.17)$$

and

$$\xi_{R,j} = \mathbf{A}_L - E\mathbf{I} - e^{iq_j}\mathbf{B}_L\ . \quad (2.18)$$

Eq. (2.16) can be generalized to more than two blob slices. If there were l blob slices each with m_{blob} atoms, the size of the generalized matrix of Eq. (2.16) is $(lm_{blob} + 2m_L) \times (lm_{blob} + 2m_L)$.

Similar to the single channel quantum dragon cases, calculating the transmission involves taking the inverse of a matrix that is usually very large. Taking the same strategy as in [16], we will map the large matrix to a smaller one. Physically, this can be seen as a transformation of the old blob to a new one, but keeping the same solution of the transmission t_{Tj}.

2.1.3 Mapping

As in [16], a mapping is searched for in order to reduce the size of the matrix in 2.16. For l blob slices, let the matrix in Eq. (2.16) be $\mathbf{N}_L$, so Eq. (2.16) is

$$\mathbf{N}_L \begin{pmatrix} \vec{\phi}_j + r_j \vec{\phi}_j^* \\ \vec{\psi}_1 \\ \vec{\psi}_2 \\ \vdots \\ \vec{\psi}_{l-1} \\ \vec{\psi}_l \\ t_{Tj}\vec{\phi}_j \end{pmatrix} = \begin{pmatrix} -2i\sin(q_j)\mathbf{B}_L^T\vec{\phi}_j \\ \vec{0} \\ \vec{0} \\ \vdots \\ \vec{0} \\ \vec{0} \\ \vec{0} \end{pmatrix} . \tag{2.19}$$

Write the mapping for $l = 2$ for brevity, then

$$\mathbf{N}_2 = \begin{pmatrix} \xi_{L,j} & -\mathbf{W} & \mathbf{0} & \mathbf{0} \\ -\mathbf{W}^T & \mathbf{A}_a - E\mathbf{I} & -\mathbf{B}_{ab} & \mathbf{0} \\ \mathbf{0} & -\mathbf{B}_{ab}^T & \mathbf{A}_b - E\mathbf{I} & -\mathbf{U} \\ \mathbf{0} & \mathbf{0} & -\mathbf{U}^T & \xi_{R,j} \end{pmatrix} . \tag{2.20}$$

Introducing transformation matrices for this two-slice nanodevice

$$\hat{\mathbf{X}}_2 = \begin{pmatrix} \mathbf{I} & & & \\ & \mathbf{X}_a & & \\ & & \mathbf{X}_b & \\ & & & \mathbf{I} \end{pmatrix} \tag{2.21}$$

and

$$\hat{\mathbf{Y}}_2 = \begin{pmatrix} \mathbf{I} & & & \\ & \mathbf{Y}_a^\dagger & & \\ & & \mathbf{Y}_b^\dagger & \\ & & & \mathbf{I} \end{pmatrix} . \tag{2.22}$$

In Eq. (2.21) and (2.22), $\mathbf{I}$ is the $m_L \times m_L$ identity matrix, the matrices $\mathbf{X}_a$ and $\mathbf{Y}_a$ are of the size $m_a \times m_a$, while $\mathbf{X}_b$ and $\mathbf{Y}_b$ are of the size $m_b \times m_b$. Blob slice a has m_a atoms, and blob slice b has m_b atoms. We have the freedom to choose the transformation matrices, as long as the X_j and Y_j are non-singular.

From Eq. (2.16)

$$\hat{\mathbf{X}}_2 \mathbf{N}_2 \hat{\mathbf{Y}}_2{}^\dagger (\hat{\mathbf{Y}}_2{}^\dagger)^{-1} \begin{pmatrix} \vec{\phi}_j + r_j \vec{\phi}_j^* \\ \vec{\psi}_a \\ \vec{\psi}_b \\ t_{Tj} \vec{\phi}_j \end{pmatrix} = \hat{\mathbf{X}}_2 \begin{pmatrix} -2i \sin(q_j) \mathbf{B}_L^T \vec{\phi}_j \\ \vec{0} \\ \vec{0} \\ \vec{0} \end{pmatrix} . \tag{2.23}$$

$$\hat{\mathbf{X}}_2\mathbf{N}_2\hat{\mathbf{Y}}_2{}^{\dagger}\begin{pmatrix}\vec{\phi}_j + r_j\vec{\phi}_j^* \\ (\mathbf{Y}_a^{\dagger})^{-1}\vec{\psi}_a \\ (\mathbf{Y}_b^{\dagger})^{-1}\vec{\psi}_b \\ t_{Tj}\vec{\phi}_j\end{pmatrix} = \begin{pmatrix}-2i\sin(q_j)\mathbf{B}_L^T\vec{\phi}_j \\ \vec{0} \\ \vec{0} \\ \vec{0}\end{pmatrix}. \quad (2.24)$$

Eq. (2.16) and Eq. (2.23) have the same solution for t_{Tj}.

Define $\mathbf{M}_l = \hat{\mathbf{X}}_l\mathbf{N}_l\hat{\mathbf{Y}}_l{}^{\dagger}$, which for $l = 2$ is

$$\mathbf{M}_2 = \begin{pmatrix}\mathbf{I} & & & \\ & \mathbf{X}_a & & \\ & & \mathbf{X}_b & \\ & & & \mathbf{I}\end{pmatrix}\begin{pmatrix}\xi_{L,j} & -\mathbf{W} & \mathbf{0} & \mathbf{0} \\ -\mathbf{W}^T & \mathbf{A}_a - E\mathbf{I} & -\mathbf{B}_{ab} & \mathbf{0} \\ \mathbf{0} & -\mathbf{B}_{ab}^T & \mathbf{A}_b - E\mathbf{I} & -\mathbf{U} \\ \mathbf{0} & \mathbf{0} & -\mathbf{U}^T & \xi_{R,j}\end{pmatrix}\begin{pmatrix}\mathbf{I} & & & \\ & \mathbf{Y}_a^{\dagger} & & \\ & & \mathbf{Y}_b^{\dagger} & \\ & & & \mathbf{I}\end{pmatrix}. \quad (2.25)$$

$$\mathbf{M}_2 = \begin{pmatrix}\xi_{L,j} & -\mathbf{W}\mathbf{Y}_a^{\dagger} & \mathbf{0} & \mathbf{0} \\ -\mathbf{X}_a\mathbf{W}^T & \mathbf{X}_a(\mathbf{A}_a - E\mathbf{I})\mathbf{Y}_a^{\dagger} & -\mathbf{X}_a\mathbf{B}_{ab}\mathbf{Y}_b^{\dagger} & \mathbf{0} \\ \mathbf{0} & -\mathbf{X}_b\mathbf{B}_{ab}^T\mathbf{Y}_a^{\dagger} & \mathbf{X}_b(\mathbf{A}_b - E\mathbf{I})\mathbf{Y}_b^{\dagger} & -\mathbf{X}_b\mathbf{U} \\ \mathbf{0} & \mathbf{0} & -\mathbf{U}^T\mathbf{Y}_b^{\dagger} & \xi_{R,j}\end{pmatrix}. \quad (2.26)$$

The $\mathbf{M}_l$ can be seen as a new matrix equation for a new nanodevice. In the previous paper [16], this transformation is called a mapping from one matrix equation to another. The new matrix equation has the same solution for the transmission t_{Tj} of channel j, as can be seen from comparison between Eq. (2.16) and Eq. (2.23). The freedom in choosing the $\hat{\mathbf{X}}_l$ and $\hat{\mathbf{Y}}_l$ will be used to try to simplify the matrix equation.

Define a successful mapping as one that satisfies the following mapping equations

$$\mathbf{X}_1\mathbf{W}^T = \begin{pmatrix}\tilde{\mathbf{W}}^T & \mathbf{0}\end{pmatrix} \quad \text{and} \quad \mathbf{W}\mathbf{Y}_1^{\dagger} = \begin{pmatrix}\tilde{\mathbf{W}}^{\dagger} \\ \mathbf{0}\end{pmatrix} \quad (2.27)$$

$$\mathbf{U}^T\mathbf{Y}_l^\dagger = \begin{pmatrix} \tilde{\mathbf{U}}^T & \mathbf{0} \end{pmatrix} \quad \text{and} \quad \mathbf{X}_l\mathbf{U} = \begin{pmatrix} \tilde{\mathbf{U}} \\ \mathbf{0} \end{pmatrix} \tag{2.28}$$

$$\mathbf{X}_j\mathbf{A}_j\mathbf{Y}_j^\dagger = \begin{pmatrix} \tilde{\mathbf{A}}_j & \mathbf{0} \\ \mathbf{0} & \hat{\mathbf{A}}_j \end{pmatrix} \tag{2.29}$$

$$E\mathbf{X}_j\mathbf{I}\mathbf{Y}_j^\dagger = \begin{pmatrix} E\mathbf{I} & \mathbf{0} \\ \mathbf{0} & \hat{\mathbf{E}} \end{pmatrix} \tag{2.30}$$

$$\mathbf{X}_j\mathbf{B}_{j,j+1}\mathbf{Y}_{j+1}^\dagger = \begin{pmatrix} \tilde{\mathbf{B}}_{j,j+1} & \mathbf{0} \\ \mathbf{0} & \hat{\mathbf{B}}_{j,j+1} \end{pmatrix} \tag{2.31}$$

$$\mathbf{X}_{j+1}\mathbf{B}_{j,j+1}^T\mathbf{Y}_j^\dagger = \begin{pmatrix} \tilde{\mathbf{B}}_{j,j+1}^T & \mathbf{0} \\ \mathbf{0} & \hat{\mathbf{B}}_{j,j+1}^T \end{pmatrix} \tag{2.32}$$

j in the Eq. (2.29) through Eq. (2.32) is the slice index of blob. For the $l = 2$ case, we have also written $j = a$ for the slice 1 and $j = b$ for the slice 2.

2.1.4 Multi-channel quantum dragons

Under the condition that a channel has a propagating wavevector q_j, the leads and blob together will be a quantum dragon if

$$\tilde{\mathbf{A}}_i = \mathbf{A}_L \quad \forall i \tag{2.33}$$

$$\tilde{\mathbf{W}} = \tilde{\mathbf{U}} = \tilde{\mathbf{B}}_{j,j+1} = \mathbf{B}_L \tag{2.34}$$

2.2 Rectangular Nanotubes

The nanodevices connected to leads can have any structure mathematically. But physically, only some structures can be experimentally realized for now. Carbon nanotubes[11] in the armchair and zigzag configurations are examples of these structures and how to find quantum dragons in these structures when connected to single chain leads are shown in [16]. In the rest of the thesis, we will focus on the nanodevices that are from rectangular lattices. Though no experimental realization of such rectangular nanotubes exist yet, these nanodevices are easier to analyze in terms of finding multi-channel quantum dragons compared to other nanotubes. Some of the ideas from analysis of rectangular nanotubes can also be used for other nanotubes.

2.2.1 Nanotubes formed from rectangular lattice

A two dimensional rectangular lattice is one of the five two dimensional Bravais lattices. The position vector $\mathbf{R}$ can be presented as

$$\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 \tag{2.35}$$

where n_i are any integers and $\mathbf{a}_i$ are the primitive vectors that span the lattice.

Rectangular nanotubes are rectangular lattices which are wrapped to tubes with zero helicity. The ease in analysis of rectangular nanotubes for multi-channel quantum dragons comes from the structure. In the slices of rectangular nanotubes, all the atom sites have the same hopping relation with the others. In other words, there is no disorder in the slices. For these rectangular nanotubes, the matrices $\mathbf{A}_i$ are circulant matrices [15][5].

A circulant matrix is an $N \times N$ matrix of a cyclic form

$$\mathbf{A} = \begin{pmatrix} a_N & a_1 & a_2 & \cdots & a_{N-1} \\ a_{N-1} & a_N & a_1 & \cdots & a_{N-2} \\ a_{N-2} & a_{N-1} & a_N & \cdots & a_{N-3} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_1 & a_2 & a_3 & \cdots & a_N \end{pmatrix} \tag{2.36}$$

where the a_k's are complex or real numbers. All the matrix elements in a given principal or secondary diagonal are the same. Circulant matrix can be symmetric or non-symmetric. The following matrices $\mathbf{A}$'s and $\mathbf{B}$'s are two examples of circulant matrices.

$$\mathbf{A}_1 = \begin{pmatrix} \epsilon & -t_1 & -t_2 & -t_3 & -t_4 & -t_3 & -t_2 & -t_1 \\ -t_1 & \epsilon & -t_1 & -t_2 & -t_3 & -t_4 & -t_3 & -t_2 \\ -t_2 & -t_1 & \epsilon & -t_1 & -t_2 & -t_3 & -t_4 & -t_3 \\ -t_3 & -t_2 & -t_1 & \epsilon & -t_1 & -t_2 & -t_3 & -t_4 \\ -t_4 & -t_3 & -t_2 & -t_1 & \epsilon & -t_1 & -t_2 & -t_3 \\ -t_3 & -t_4 & -t_3 & -t_2 & -t_1 & \epsilon & -t_1 & -t_2 \\ -t_2 & -t_3 & -t_4 & -t_3 & -t_2 & -t_1 & \epsilon & -t_1 \\ -t_1 & -t_2 & -t_3 & -t_4 & -t_3 & -t_2 & -t_1 & \epsilon \end{pmatrix} \tag{2.37}$$

where t_i are non-negative real numbers and ϵ is a positive number.

Elements of the matrix can also be zero

$$\mathbf{A}_2 = \begin{pmatrix} \epsilon & -t_1 & 0 & -t_3 & 0 & -t_3 & -t_2 & -t_1 \\ -t_1 & \epsilon & -t_1 & 0 & -t_3 & 0 & -t_3 & -t_2 \\ -t_2 & -t_1 & \epsilon & -t_1 & 0 & -t_3 & 0 & -t_3 \\ -t_3 & -t_2 & -t_1 & \epsilon & -t_1 & 0 & -t_3 & 0 \\ 0 & -t_3 & -t_2 & -t_1 & \epsilon & -t_1 & 0 & -t_3 \\ -t_3 & 0 & -t_3 & -t_2 & -t_1 & \epsilon & -t_1 & 0 \\ 0 & -t_3 & 0 & -t_3 & -t_2 & -t_1 & \epsilon & -t_1 \\ -t_1 & 0 & -t_3 & 0 & -t_3 & -t_2 & -t_1 & \epsilon \end{pmatrix}. \tag{2.38}$$

$\mathbf{A}_1$ and $\mathbf{A}_2$ can be associated with the matrices that represent the intra-slice hopping in each slice of the nanotubes.

$$\mathbf{B}_1 = \begin{pmatrix} -s_0 & -s_1 & -s_2 & -s_3 & -s_4 \\ -s_4 & -s_0 & -s_1 & -s_2 & -s_3 \\ -s_3 & -s_4 & -s_0 & -s_1 & -s_2 \\ -s_2 & -s_3 & -s_4 & -s_0 & -s_1 \\ -s_1 & -s_2 & -s_3 & -s_4 & -s_0 \end{pmatrix}. \tag{2.39}$$

$$\mathbf{B}_2 = \begin{pmatrix} -s_0 & 0 & 0 & 0 & 0 \\ 0 & -s_0 & 0 & 0 & 0 \\ 0 & 0 & -s_0 & 0 & 0 \\ 0 & 0 & 0 & -s_0 & 0 \\ 0 & 0 & 0 & 0 & -s_0 \end{pmatrix}. \tag{2.40}$$

$\mathbf{B}_1$ and $\mathbf{B}_2$ can be the associated matrices that represent the inter-slice hopping between each slice of a rectangular nanotube.

Introduce a single permutation matrix $\mathbf{P}$

$$\mathbf{P} = \begin{pmatrix} 0 & 1 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 0 & 0 & 0 & \cdots & 0 \end{pmatrix} . \tag{2.41}$$

which comes from a permutation π of m elements

$$\pi : \{1, 2, \ldots, N-1, N\} \to \{2, 3, \ldots, N, 1\} . \tag{2.42}$$

The general form of circulant matrices can be written as a polynomial in $\mathbf{P}$

$$\mathbf{A} = a_1\mathbf{P} + a_2\mathbf{P^2} + a_3\mathbf{P^3} + \cdots + a_N\mathbf{P^N} . \tag{2.43}$$

All the integer powers of $\mathbf{P}$ have the same eigenvector with $\mathbf{P}$ but with a different eigenvalues. Consider a single permutation matrix $\mathbf{P}_n$

$$\mathbf{P}_n = \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 0 & 0 & \cdots & 0 \end{pmatrix} \tag{2.44}$$

The n's eigenvalues of matrix $\mathbf{P}_n$ are

$$e^{j2\pi i/n} \tag{2.45}$$

where $j = 0, 1, \cdots, n-1$.

The associated eigenvectors with eigenvalues $e^{j2\pi i/n}$ are

$$\frac{1}{\sqrt{n}} \begin{pmatrix} e^{\frac{j0\,2\pi i}{n}} \\ e^{\frac{j1\,2\pi i}{n}} \\ \vdots \\ e^{\frac{j(n-1)\,2\pi i}{n}} \end{pmatrix} . \tag{2.46}$$

Therefore a circulant matrix can be diagonalized by a finite Fourier transform since the eigenvalues of the permutation matrix $\mathbf{P}$ are the N_i roots of unity and the eigenvectors of $\mathbf{P}$ also have its elements as a normalization times a root of unity. This property will be used in the analysis of finding multi-channel quantum dragons in later chapter.

CHAPTER 3

EXAMPLE MULTI-CHANNEL QUANTUM DRAGONS IN RECTANGULAR NANOTUBES

3.1 Example solution for 2 channels lead connected to 4 channels blob: 2:4:2 Structure

It is shown in this section how to find multi-channel quantum dragons from rectangular nanotubes. Specifically, the blob and leads are rectangular nanotubes consisting of identical slices.

Assume the rectangular nanotube blob has four atoms in each slice with the intra-slice matrix of the form.

$$\mathbf{A}_l = \begin{pmatrix} \epsilon & -t_1 & -t_2 & -t_1 \\ -t_1 & \epsilon & -t_1 & -t_2 \\ -t_2 & -t_1 & \epsilon & -t_1 \\ -t_1 & -t_2 & -t_1 & \epsilon \end{pmatrix} \tag{3.1}$$

where ϵ is the on-site energy for the atoms and the t's are the hopping parameters between atoms. These symbols are also used to present the same physical quantities in the rest of the thesis.

[1]Blue points represent atoms in a rectangular nanotube slice. Yellow lines represent the nearest neighbor hopping $-t_1$. Green lines represent the next-to-nearest neighbor hopping $-t_2$. All atoms are located in the xy plane.

[2]All the intra-slice hopping terms have been shown as yellow and green lines.

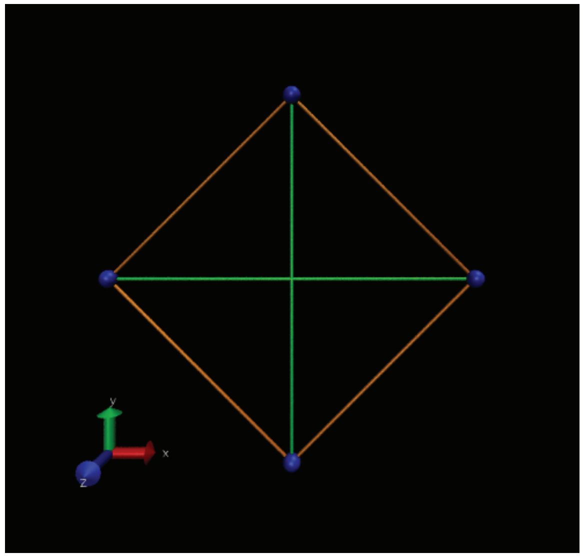

Figure 3.1: The diagram for the matrix in Eq. (3.1).[1]

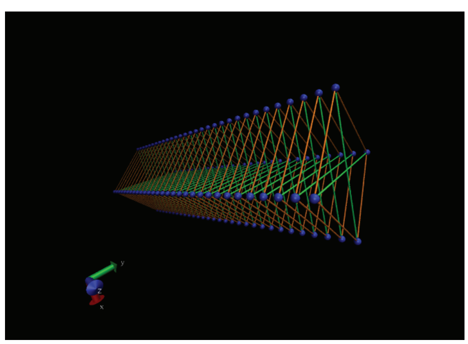

Figure 3.2: The diagram for a blob consisting of 30 identical slices from Eq. (3.1).[2]

Assume that the rectangular nanotube lead intra-slice matrix is of the form

$$\mathbf{A}_L = \begin{pmatrix} \sigma & -t_{11} \\ -t_{11} & \sigma \end{pmatrix} . \tag{3.2}$$

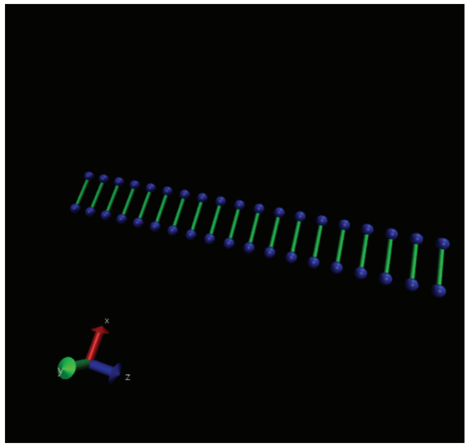

Figure 3.3: The diagram for a lead consisting of 19 identical slices from Eq. (3.2).[3]

Assume that the blob inter-slice matrix and lead inter-slice are both identity matrices of different dimensions

$$\mathbf{B}_l = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} . \tag{3.3}$$

$$\mathbf{B}_L = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} . \tag{3.4}$$

[3]Since there are only 2 atoms in each slice, only nearest neighbor hopping terms exists and are shown as green lines.

[4]Red lines indicate the only inter-slice hopping between nearest neighbor atom sites from two successive slices.

[5]Yellow lines indicate the only inter-slice hopping between nearest neighbor atom sites from two successive slices.

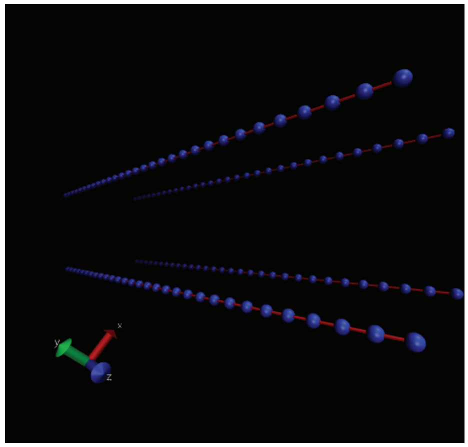

Figure 3.4: The diagram for inter-slice hopping shown in Eq. (3.3).[4]

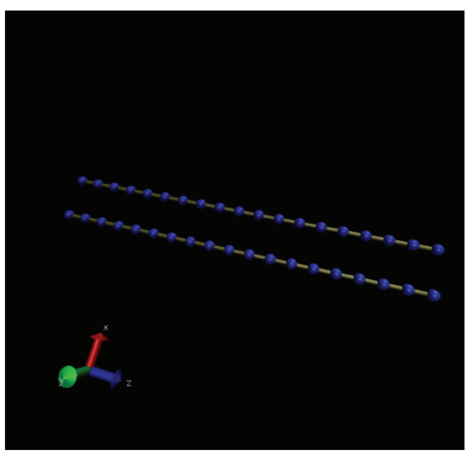

Figure 3.5: The diagram for inter-slice hopping shown in Eq. (3.4).[5]

In this example, all the slices in the leads and the blob are the same. This means that the same transformation matrices $\mathbf{X}$ and $\mathbf{Y}$ can be used for the mapping of all slices in blob. To find multi-channel quantum dragons, the transformation matrix for a successful mapping should be found first.

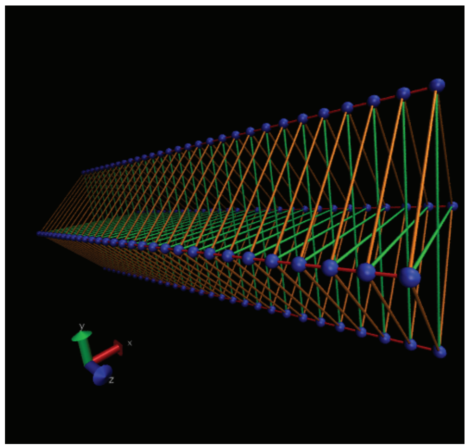

Figure 3.6: The diagram shows both intra-slice and inter-slice hopping bonds in the blob.[6]

Since in this example, a 4 atom per slice rectangular nanotube blob is connected to 2 atom per slice rectangular leads. The connection matrix $\mathbf{W}$ is 2×4 in size.

$$\mathbf{W} = \begin{pmatrix} w_{11} & w_{12} & w_{13} & w_{14} \\ w_{21} & w_{22} & w_{23} & w_{24} \end{pmatrix} \tag{3.5}$$

where the w_{ij} are hopping terms between lead a slice and a blob slice. The i index is for the atoms in lead. Since there are 2 atoms in each lead slice , i can be 1 or 2.The j index is for the atoms in the blob, j can be 1,2,3 or 4 since there are 4 atoms in each blob slice.

[6]This diagram consists of 30 blob slices. Blue points indicate atoms and different color lines indicate different hopping terms.

[7]Leads are semi-infinite but only finite slices are shown in the diagram. All the hopping terms are not shown. In the following section, the hopping parameters in each matrix are tuned to turn the blob into a multi-channel quantum dragon.

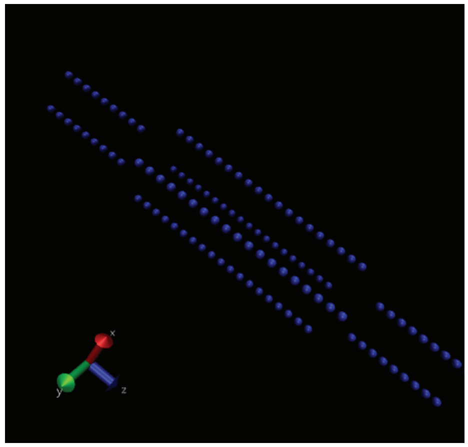

Figure 3.7: A 19 slices rectangular nanotube blob and the incoming and outgoing leads.[7]

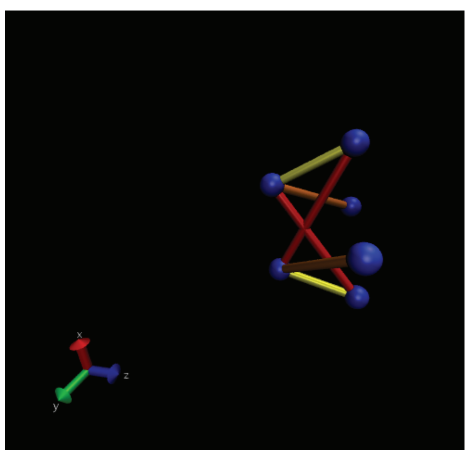

Figure 3.8: Connection between blob slice and lead slice.[8]

Assume that the transformation matrices $\mathbf{X}$ and $\mathbf{Y}$ are the same. Furthermore, assume that $\mathbf{W}$ is equal to $\mathbf{U}^T$, this means that the connection between the last slice in the incoming lead to the first slice of the blob and the connection between the last slice in the blob to the first slice in the outgoing lead are the same. After making these assumptions, the set of successful mapping equations in Eq. (2.27) to Eq. (2.32) become

$$\mathbf{W}\mathbf{X}_1^\dagger = \begin{pmatrix} \tilde{\mathbf{W}} & \mathbf{0} \end{pmatrix} . \tag{3.6}$$

$$\mathbf{X}_j\mathbf{A}_j\mathbf{X}_j^\dagger = \begin{pmatrix} \tilde{\mathbf{A}}_j & \mathbf{0} \\ \mathbf{0} & \hat{\mathbf{A}}_j \end{pmatrix} . \tag{3.7}$$

$$\mathbf{X}_j\mathbf{B}_{j,j+1}\mathbf{X}_{j+1}^\dagger = \begin{pmatrix} \tilde{\mathbf{B}}_{j,j+1} & \mathbf{0} \\ \mathbf{0} & \hat{\mathbf{B}}_{j,j+1} \end{pmatrix} . \tag{3.8}$$

where j is the blob slice index.

Circulant matrices can be diagonalized by the eigenvectors of the matrix

$$\mathbf{P^1} + \mathbf{P^{-1}} = \begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{pmatrix} . \tag{3.9}$$

[8] Connection between the first slice of the blob and the last slice of the incoming lead. All the hopping terms between atoms in the lead and atoms in the blob are shown as different color lines.

The transpose conjugate eigenvectors are

$$\begin{aligned}
\mathbf{V}_1^{4\dagger} &= \begin{pmatrix} -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \end{pmatrix} \\
\mathbf{V}_2^{4\dagger} &= \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{pmatrix} \\
\mathbf{V}_3^{4\dagger} &= \begin{pmatrix} 0 & -\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \end{pmatrix} \\
\mathbf{V}_4^{4\dagger} &= \begin{pmatrix} -\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 \end{pmatrix}
\end{aligned} . \tag{3.10}$$

where the superscript is the index of the dimension of the vectors and the subscript index is the number of the vectors.

Let $\mathbf{X}_{map}$ to be set to

$$\mathbf{X}_{map} = \begin{pmatrix} \mathbf{V}_1^{4\dagger} \\ \mathbf{V}_2^{4\dagger} \\ \mathbf{V}_3^{4\dagger} \\ \mathbf{V}_4^{4\dagger} \end{pmatrix} . \tag{3.11}$$

Since $\mathbf{X}_{map}$ is a unitary matrix, we can diagonalize $\mathbf{A}_l$

$$\mathbf{X}_{map}\mathbf{A}_l\mathbf{X}_{map}^{\dagger} = \mathbf{A}_{diagonal} . \tag{3.12}$$

$$\mathbf{A}_{diagonal} = \begin{pmatrix} 2t_1 - t_2 + \epsilon & 0 & 0 & 0 \\ 0 & -2t_1 - t_2 + \epsilon & 0 & 0 \\ 0 & 0 & t_2 + \epsilon & 0 \\ 0 & 0 & 0 & t_2 + \epsilon \end{pmatrix} . \tag{3.13}$$

Let $\mathbf{X} = \mathbf{X}_{new}\mathbf{X}_{map}$

$$\mathbf{X}\mathbf{A}_l\mathbf{X}^{\dagger} = \begin{pmatrix} \tilde{\mathbf{A}} & \mathbf{0} \\ \mathbf{0} & \hat{\mathbf{A}} \end{pmatrix} . \tag{3.14}$$

$$\mathbf{X}_{new}\mathbf{X}_{map}\mathbf{A}_l\mathbf{X}_{map}^{\dagger}\mathbf{X}_{new}^{\dagger} = \begin{pmatrix} \tilde{\mathbf{A}} & \mathbf{0} \\ \mathbf{0} & \hat{\mathbf{A}} \end{pmatrix} . \tag{3.15}$$

Assume

$$\mathbf{X}_{new} = \begin{pmatrix} \mathbf{X}_{block} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{pmatrix} \tag{3.16}$$

where $\mathbf{X}_{block}$ is a 2×2 unitary matrix.

Then

$$\begin{pmatrix} \mathbf{X}_{block} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{pmatrix} \begin{pmatrix} 2t_1 - t_2 + \epsilon & 0 & 0 & 0 \\ 0 & -2t_1 - t_2 + \epsilon & 0 & 0 \\ 0 & 0 & t_2 + \epsilon & 0 \\ 0 & 0 & 0 & t_2 + \epsilon \end{pmatrix} \begin{pmatrix} \mathbf{X}_{block}^{\dagger} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{pmatrix} . \tag{3.17}$$

$$= \begin{pmatrix} \tilde{\mathbf{A}} & \mathbf{0} \\ \mathbf{0} & \hat{\mathbf{A}} \end{pmatrix}$$

To have multi-channel dragons,

$$\tilde{\mathbf{A}} = \mathbf{A}_L = \begin{pmatrix} \sigma & -t_{11} \\ -t_{11} & \sigma \end{pmatrix} . \tag{3.18}$$

From Eq. (3.17)

$$\begin{pmatrix} 2t_1 - t_2 + \epsilon & 0 & 0 & 0 \\ 0 & -2t_1 - t_2 + \epsilon & 0 & 0 \\ 0 & 0 & t_2 + \epsilon & 0 \\ 0 & 0 & 0 & t_2 + \epsilon \end{pmatrix} . \tag{3.19}$$

$$= \begin{pmatrix} \mathbf{X}^{\dagger}_{block} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{pmatrix} \begin{pmatrix} \tilde{\mathbf{A}} & \mathbf{0} \\ \mathbf{0} & \hat{\mathbf{A}} \end{pmatrix} \begin{pmatrix} \mathbf{X}_{block} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{pmatrix}$$

$$\begin{pmatrix} \mathbf{X}^{\dagger}_{block} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{pmatrix} \begin{pmatrix} \tilde{\mathbf{A}} & \mathbf{0} \\ \mathbf{0} & \hat{\mathbf{A}} \end{pmatrix} \begin{pmatrix} \mathbf{X}_{block} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{pmatrix} = \begin{pmatrix} \mathbf{X}^{\dagger}_{block}\tilde{\mathbf{A}}\mathbf{X}_{block} & 0 \\ 0 & \hat{\mathbf{A}} \end{pmatrix} . \tag{3.20}$$

Since $\mathbf{A}_L$ and $\tilde{\mathbf{A}}$ are circulant matrices, they can be diagonalized by the eigenvectors of the matrix

$$\mathbf{P}^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} . \tag{3.21}$$

The transpose of the eigenvectors are

$$\begin{aligned} \mathbf{V}_1^{2\dagger} &= \begin{pmatrix} -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \\ \mathbf{V}_2^{2\dagger} &= \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \end{aligned} . \tag{3.22}$$

Let

$$\mathbf{X}^{\dagger}_{block} = \begin{pmatrix} \mathbf{V}_1^{2\dagger} \\ \mathbf{V}_2^{2\dagger} \end{pmatrix} . \tag{3.23}$$

Then

$$\mathbf{X}^{\dagger}_{block}\tilde{\mathbf{A}}\mathbf{X}_{block} = \begin{pmatrix} \sigma + t_{11} & 0 \\ 0 & \sigma - t_{11} \end{pmatrix} . \tag{3.24}$$

From Eq. (3.19)

$$\begin{aligned} 2t_1 - t_2 + \epsilon &= \sigma + t_{11} \\ -2t_1 - t_2 + \epsilon &= \sigma - t_{11} \end{aligned} . \tag{3.25}$$

So one has

$$\begin{aligned} \sigma &= \epsilon - t_2 \\ t_{11} &= 2t_1 \end{aligned} . \tag{3.26}$$

That is, if the parameters in the lead matrix are chosen as Eq. (3.26), the mapping equation Eq. (3.7) is satisfied. Now move to the next mapping equation Eq.(3.6).

The transformation matrix $\mathbf{X}$ is

$$\mathbf{X} = \mathbf{X}_{new}\mathbf{X}_{map} . \tag{3.27}$$

Substitute $\mathbf{X}$ back into Eq. (3.6)

$$\mathbf{W}\mathbf{X}^{\dagger} = \begin{pmatrix} \tilde{\mathbf{W}} & \mathbf{0} \end{pmatrix} . \tag{3.28}$$

Hence

$$\mathbf{W}\mathbf{X}^{\dagger}_{map}\mathbf{X}^{\dagger}_{new} = \begin{pmatrix} \tilde{\mathbf{W}} & \mathbf{0} \end{pmatrix} . \tag{3.29}$$

To have multi-channel dragons, set $\tilde{\mathbf{W}} = \mathbf{B}_L$.

Assume

$$\mathbf{W} = \begin{pmatrix} b_{11}\mathbf{V}_1^{4\dagger} + b_{12}\mathbf{V}_2^{4\dagger} \\ b_{21}\mathbf{V}_1^{4\dagger} + b_{22}\mathbf{V}_2^{4\dagger} \end{pmatrix} . \tag{3.30}$$

Substitute $\mathbf{W}$ back into the mapping equation.

$$\begin{aligned}
&\mathbf{W}\mathbf{X}^{\dagger} \\
=&\mathbf{W}\mathbf{X}^{\dagger}_{map}\mathbf{X}^{\dagger}_{new} \\
=&\begin{pmatrix} b_{11}\mathbf{V}_1^{4\dagger} + b_{12}\mathbf{V}_2^{4\dagger} \\ b_{21}\mathbf{V}_1^{4\dagger} + b_{22}\mathbf{V}_2^{4\dagger} \end{pmatrix} \begin{pmatrix} \mathbf{V}_1^4 & \mathbf{V}_2^4 & \mathbf{V}_3^4 & \mathbf{V}_4^4 \end{pmatrix} \begin{pmatrix} \begin{pmatrix} \mathbf{V}_1^{2\dagger} \\ \mathbf{V}_2^{2\dagger} \end{pmatrix} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{pmatrix} \\
=&\begin{pmatrix} b_{11} & b_{12} & 0 & 0 \\ b_{21} & b_{22} & 0 & 0 \end{pmatrix} \begin{pmatrix} \begin{pmatrix} \mathbf{V}_1^{2\dagger} \\ \mathbf{V}_2^{2\dagger} \end{pmatrix} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{pmatrix} \\
=&\begin{pmatrix} \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} \begin{pmatrix} \mathbf{V}_1^{2\dagger} \\ \mathbf{V}_2^{2\dagger} \end{pmatrix} & \mathbf{0} \end{pmatrix} .
\end{aligned} \tag{3.31}$$

Set

$$\begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} \begin{pmatrix} \mathbf{V}_1^{2\dagger} \\ \mathbf{V}_2^{2\dagger} \end{pmatrix} = \mathbf{B}_L = \mathbf{I} \, . \tag{3.32}$$

The b's can be solved as

$$\begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} = \begin{pmatrix} \mathbf{V}_1^2 & \mathbf{V}_2^2 \end{pmatrix} = \begin{pmatrix} -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} . \tag{3.33}$$

Combine Eq. (3.33) and Eq. (3.30) to give

$$\mathbf{W} = \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \end{pmatrix} . \tag{3.34}$$

[9] To better show the connection, the atoms in the first slice of the blob are shown in yellow.

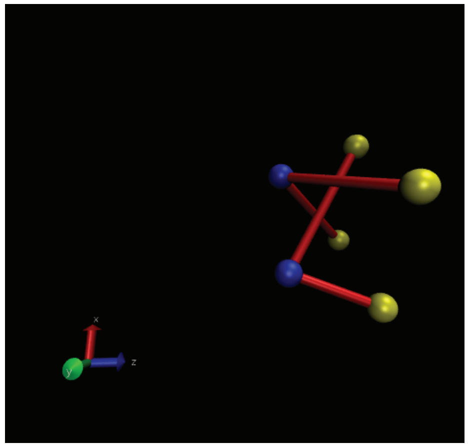

Figure 3.9: The diagram shows the lead-slice connection $\mathbf{W}$ from Eq.(3.34).[9]

The last mapping equation to be satisfied is Eq. (3.8)

$$\mathbf{X}_j \mathbf{B}_{j,j+1} \mathbf{X}_{j+1}^{\dagger} = \begin{pmatrix} \tilde{\mathbf{B}}_{j,j+1} & \mathbf{0} \\ \mathbf{0} & \hat{\mathbf{B}}_{j,j+1} \end{pmatrix} . \tag{3.35}$$

Use $\mathbf{X}$ in Eq. (3.27), $\mathbf{B}_l$ in Eq. (3.3) and $\mathbf{B}_L$ in Eq. (3.4), a successful mapping is automatically satisfied. The condition to have multi-channel dragons is $\tilde{\mathbf{B}}_{j,j+1} = \mathbf{B}_L$, which is also automatically satisfied.

So all the mapping equations in Eq. (3.6) to Eq. (3.8) are satisfied with the $\mathbf{A}_L$, $\mathbf{A}_l$, $\mathbf{B}_L$, $\mathbf{B}_l$, and $\mathbf{W}$ in Eq. (3.34), and results in Eq. (3.44). If a rectangular blob is connected to rectangular leads, where both the blob and lead come from $\mathbf{A}_L$ in Eq. (3.2) , $\mathbf{A}_l$ in Eq. (3.2) , $\mathbf{B}_L$ in Eq. (3.4) , $\mathbf{B}_l$ in Eq. (3.3) , and $\mathbf{W}$ in Eq. (3.30) , this blob will be a multi-channel quantum dragon.

After a multi-channel quantum dragon is found, it can have multiple open channels with total transmission. But depending on the actual values that the parameters in these

[10]The diagram shows a multi-channel quantum dragon with a 4 atoms per slice rectangular nanotube blob connected to 2 atoms per slice rectangular nanotube leads.There are 19 identical slices in the blob.

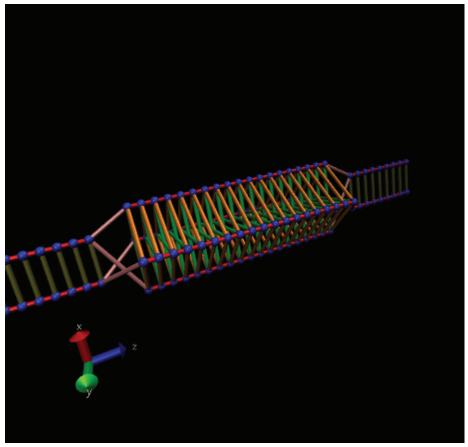

Figure 3.10: A 2:4:2 multi-channel quantum dragon.[10]

matrices are chosen to be, the energy ranges for open transmission in each channel are different.

The eigen equation to solve for the energy ranges for each mode is

$$[-\mathbf{B}_L^T e^{-iq} + (\mathbf{A}_L - E\mathbf{I}) - \mathbf{B}_L e^{iq}]\vec{\phi}_j = \lambda_j(E,q)\vec{\phi}_j \tag{3.36}$$

with

$$\lambda_j(E,q) = 0\,. \tag{3.37}$$

Substitute the $\mathbf{A}_L$ in Eq. (3.2) and $\mathbf{B}_L$ in Eq. (3.4) back into Eq. (3.36) to give

$$[\sigma\mathbf{I} - t_{11}\mathbf{P}^1 - E\mathbf{I} - 2\cos q\mathbf{I}]\vec{\phi}_j = \lambda_j(E,q)\vec{\phi}_j \tag{3.38}$$

where $\mathbf{P}^1$ is the single permutation matrix of dimension 2×2.

Since the eigenvalues and eigenvectors of permutation matrices are known from the discussion of circulant matrices , the eigenvalues of Eq.(3.38) can be easily found

$$\begin{aligned} \lambda_1 &= \sigma - 2\cos q_1 - t_{11} - E \\ \lambda_2 &= \sigma - 2\cos q_2 + t_{11} - E \end{aligned}\,. \tag{3.39}$$

Set the eigenvalues to be zero , which gives

$$\begin{aligned}\cos q_1 &= \frac{1}{2}(\sigma - t_{11} - E) \\ \cos q_2 &= \frac{1}{2}(\sigma + t_{11} - E)\end{aligned} . \tag{3.40}$$

Since $-1 \leq \cos q \leq 1$

$$\begin{aligned}\sigma - t_{11} - 2 \leq &E \leq \sigma - t_{11} + 2 \\ \sigma + t_{11} - 2 \leq &E \leq \sigma + t_{11} + 2\end{aligned} . \tag{3.41}$$

Provided that t_{11} is non-negative, to have 2 channels open simultaneously, the following condition should be satisfied

$$\begin{aligned}\sigma + t_{11} - 2 < \sigma - t_{11} + 2 \\ t_{11} < 2\end{aligned} . \tag{3.42}$$

After multi-channel quantum dragons are found in this 2 atoms slice lead and 4 atoms slice blob setting, a matrix method for transmission calculation is used to validate the results. In this validation calculation, the blob consists of 4 slices. For each mode q, the transmission is solved. All the transmissions are 1 in uints of G_0 using the result in this section. Also if Eq. (3.42) is satisfied, two channels can be opened simultaneously.

[11]The diagram shows a multi-channel quantum dragon from a 4 atoms per slice rectangular nanotube blob connected to a 2 atoms per slice rectangular nanotube lead. The conductance is calculated from the matrix method. There are 4 slices in the blob put into the matrix. It can be seen that the two channels have different energy ranges. The matrix parameters have been set as follows: $\epsilon = 3$, $t_1 = 3$, and $t_2 = 2$, which gives $\sigma = 1$ and $t_{11} = 6$.

[12]The diagram shows a multi-channel quantum dragon from 4 atoms per slice rectangular nanotube blob connected to a 2 atoms per slice rectangular nanotube lead. The conductance is calculated from the matrix method. There are 4 slices in the blob put into the the matrix. The matrix parameters have been set as follows: $\epsilon = 3$, $t_1 = 0.5$, and $t_2 = 0.3$, which gives $\sigma = 2.7$ and $t_{11} = 1$. Since the parameters are tuned to satisfy Eq.(3.42), the two energy ranges have some overlap, which means that in this overlap energy, these two channels can have total transmission open simultaneously.

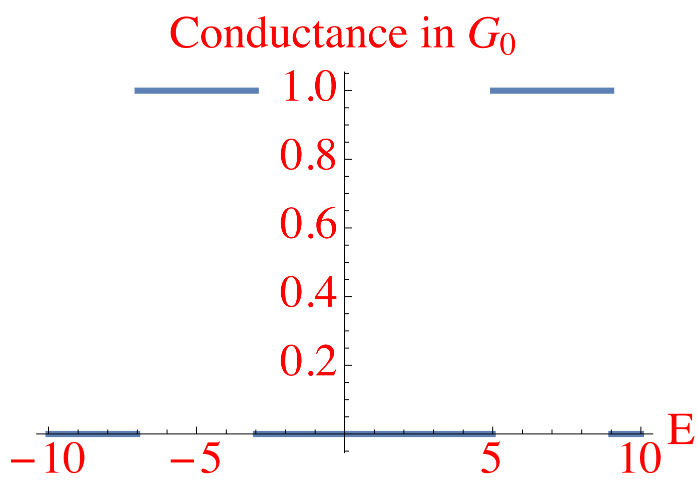

Figure 3.11: Conductance from 2:4:2 quantum dragons: 1 open channels case[11]

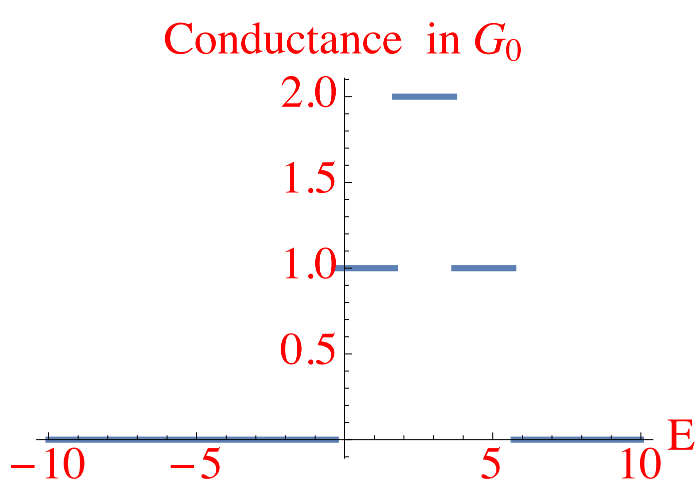

Figure 3.12: Conductance from 2:4:2 quantum dragons: 2 open channels case[12]

3.2 Example solution for a 4 atoms per slice lead connected to an 8 atoms per slice blob: 4:8:4 Structure

In this subsection, an example of multi-channel quantum dragons from a 8 atoms per slice rectangular blob connected to 4 atoms per slice rectangular leads is shown. The general method applied here is the same as in last subsection. Assume the rectangular blob intra-slice matrix is

$$\mathbf{A}_l = \begin{pmatrix} \epsilon & -t_1 & -t_2 & -t_3 & -t_4 & -t_3 & -t_2 & -t_1 \\ -t_1 & \epsilon & -t_1 & -t_2 & -t_3 & -t_4 & -t_3 & -t_2 \\ -t_2 & -t_1 & \epsilon & -t_1 & -t_2 & -t_3 & -t_4 & -t_3 \\ -t_3 & -t_2 & -t_1 & \epsilon & -t_1 & -t_2 & -t_3 & -t_4 \\ -t_4 & -t_3 & -t_2 & -t_1 & \epsilon & -t_1 & -t_2 & -t_3 \\ -t_3 & -t_4 & -t_3 & -t_2 & -t_1 & \epsilon & -t_1 & -t_2 \\ -t_2 & -t_3 & -t_4 & -t_3 & -t_2 & -t_1 & \epsilon & -t_1 \\ -t_1 & -t_2 & -t_3 & -t_4 & -t_3 & -t_2 & -t_1 & \epsilon \end{pmatrix} . \tag{3.43}$$

The rectangular lead intra-slice matrix is

$$\mathbf{A}_L = \begin{pmatrix} \sigma & -t_{11} & -t_{22} & -t_{11} \\ -t_{11} & \sigma & -t_{11} & -t_{22} \\ -t_{22} & -t_{11} & \sigma & -t_{11} \\ -t_{11} & -t_{22} & -t_{11} & \sigma \end{pmatrix} . \tag{3.44}$$

Let the blob inter-slice matrix and the lead inter-slice matrix be identity matrices of appropriate dimensions.

$$\mathbf{B}_l = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} . \tag{3.45}$$

$$\mathbf{B}_L = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} . \tag{3.46}$$

To have a multi channel quantum dragon, the Eq. (3.6), Eq. (3.7) and Eq. (3.8) should be satisfied.

The eigenvectors used to diagonalize this matrix are the eigenvectors of matrix

$$\mathbf{P}^1 + \mathbf{P}^{-1} = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix} . \tag{3.47}$$

The transpose conjugate of the 8 eigenvectors are

$$\begin{aligned}
\mathbf{V_1^{8\dagger}} &= \begin{pmatrix} -\frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} & -\frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} & -\frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} & -\frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} \end{pmatrix} \\
\mathbf{V_2^{8\dagger}} &= \begin{pmatrix} \frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} & \frac{1}{2\sqrt{2}} \end{pmatrix} \\
\mathbf{V_3^{8\dagger}} &= \begin{pmatrix} 0 & -\frac{1}{2} & 0 & \frac{1}{2} & 0 & -\frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix} \\
\mathbf{V_4^{8\dagger}} &= \begin{pmatrix} -\frac{1}{2} & 0 & \frac{1}{2} & 0 & -\frac{1}{2} & 0 & \frac{1}{2} & 0 \end{pmatrix} \\
\mathbf{V_5^{8\dagger}} &= \begin{pmatrix} \frac{1}{2} & \frac{1}{2\sqrt{2}} & 0 & -\frac{1}{2\sqrt{2}} & -\frac{1}{2} & -\frac{1}{2\sqrt{2}} & 0 & \frac{1}{2\sqrt{2}} \end{pmatrix} \\
\mathbf{V_6^{8\dagger}} &= \begin{pmatrix} 0 & -\frac{1}{2\sqrt{2}} & -\frac{1}{2} & -\frac{1}{2\sqrt{2}} & 0 & \frac{1}{2\sqrt{2}} & \frac{1}{2} & \frac{1}{2\sqrt{2}} \end{pmatrix} \\
\mathbf{V_7^{8\dagger}} &= \begin{pmatrix} -\frac{1}{2} & \frac{1}{2\sqrt{2}} & 0 & -\frac{1}{2\sqrt{2}} & \frac{1}{2} & -\frac{1}{2\sqrt{2}} & 0 & \frac{1}{2\sqrt{2}} \end{pmatrix} \\
\mathbf{V_8^{8\dagger}} &= \begin{pmatrix} 0 & \frac{1}{2\sqrt{2}} & -\frac{1}{2} & \frac{1}{2\sqrt{2}} & 0 & -\frac{1}{2\sqrt{2}} & \frac{1}{2} & -\frac{1}{2\sqrt{2}} \end{pmatrix}
\end{aligned} . \tag{3.48}$$

Put each eigenvector as rows in the $\mathbf{X_{map}}$, so the blob matrix can be diagonalized.

$$\mathbf{X_{map}} = \begin{pmatrix} \mathbf{V_1^{8\dagger}} \\ \mathbf{V_2^{8\dagger}} \\ \mathbf{V_3^{8\dagger}} \\ \mathbf{V_4^{8\dagger}} \\ \mathbf{V_5^{8\dagger}} \\ \mathbf{V_6^{8\dagger}} \\ \mathbf{V_7^{8\dagger}} \\ \mathbf{V_8^{8\dagger}} \end{pmatrix} . \tag{3.49}$$

$$\mathbf{X_{map}} \mathbf{A_{blob}} (\mathbf{X_{map}})^{\dagger} = \mathbf{A_{diagonal}} . \tag{3.50}$$

The diagonalized matrix $\mathbf{A_{diagonal}}$ is

$$\mathbf{A_{diagonal}} = \begin{pmatrix} \alpha & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \beta & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \gamma & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \gamma & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \eta & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \eta & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \mu & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \mu \end{pmatrix} . \tag{3.51}$$

Here

$$\begin{aligned}
&\alpha = 2t_1 - 2t_2 + 2t_3 - t_4 + \epsilon \\
&\beta = -2t_1 - 2t_2 - 2t_3 - t_4 + \epsilon \\
&\gamma = 2t_2 - t_4 + \epsilon \qquad\qquad\qquad . \\
&\eta = -\sqrt{2}t_1 + \sqrt{2}t_3 + t_4 + \epsilon \\
&\mu = \sqrt{2}t_1 - \sqrt{2}t_3 + t_4 + \epsilon
\end{aligned} \tag{3.52}$$

Let $\mathbf{X} = \mathbf{X_{new}}\mathbf{X_{map}}$

$$\mathbf{X_{new}}\mathbf{X_{map}}\mathbf{A}\mathbf{X_{map}^{\dagger}}\mathbf{X_{new}^{\dagger}} = \begin{pmatrix} \tilde{\mathbf{A}} & \mathbf{0} \\ \mathbf{0} & \hat{\mathbf{A}} \end{pmatrix} . \tag{3.53}$$

$$\mathbf{X_{new}}\mathbf{A_{diagonal}}\mathbf{X_{new}^{\dagger}} = \begin{pmatrix} \tilde{\mathbf{A}} & \mathbf{0} \\ \mathbf{0} & \hat{\mathbf{A}} \end{pmatrix} . \tag{3.54}$$

Assume that $\mathbf{X_{new}}$ is unitary. From the above equation we can have the following equation

$$\mathbf{A_{diagonal}} = \mathbf{X_{new}^{\dagger}} \begin{pmatrix} \tilde{\mathbf{A}} & \mathbf{0} \\ \mathbf{0} & \hat{\mathbf{A}} \end{pmatrix} \mathbf{X_{new}} . \tag{3.55}$$

$\tilde{\mathbf{A}}$ should be the same as $\mathbf{A}_L$

$$\tilde{\mathbf{A}} = \mathbf{A}_L = \begin{pmatrix} \sigma & -t_{11} & -t_{22} & -t_{11} \\ -t_{11} & \sigma & -t_{11} & -t_{22} \\ -t_{22} & -t_{11} & \sigma & -t_{11} \\ -t_{11} & -t_{22} & -t_{11} & \sigma \end{pmatrix} . \tag{3.56}$$

Assume $\mathbf{X_{new}}$ has the block matrix form

$$\mathbf{X_{new}} = \begin{pmatrix} \mathbf{X_{block}} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{pmatrix} . \tag{3.57}$$

This gives

$$\mathbf{A_{diagonal}} = \begin{pmatrix} \mathbf{X_{block}}^{\dagger} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{pmatrix} \begin{pmatrix} \tilde{\mathbf{A}} & \mathbf{0} \\ \mathbf{0} & \hat{\mathbf{A}} \end{pmatrix} \begin{pmatrix} \mathbf{X_{block}} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{pmatrix} . \tag{3.58}$$

$$\mathbf{A_{diagonal}} = \begin{pmatrix} \mathbf{X_{block}}^{\dagger}\tilde{\mathbf{A}}\mathbf{X_{block}} & \mathbf{0} \\ \mathbf{0} & \hat{\mathbf{A}} \end{pmatrix} . \tag{3.59}$$

So the $\mathbf{X_{block}}$ matrix maps the lead matrix $\tilde{\mathbf{A}}$ to the eigenvalues of the blob matrix. Using this equation, the hopping parameters and on-site energy of the lead matrix can be solved in terms of hopping parameters and on-site energy from the blob matrix. Since $\tilde{\mathbf{A}}$ is a rectangular matrix, it can also be diagonalized by the eigenvectors of the matrix

$$\mathbf{P}^{1} + \mathbf{P}^{-1} = \begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{pmatrix} . \tag{3.60}$$

So one has

$$\mathbf{X_{block}}^{\dagger} = \begin{pmatrix} -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ 0 & -\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 \end{pmatrix} . \tag{3.61}$$

By choosing this $\mathbf{X_{block}}^\dagger$, $\mathbf{X_{block}}^\dagger\tilde{\mathbf{A}}\mathbf{X_{block}}$ becomes

$$\begin{pmatrix} 2t_{11}-t_{22}+\sigma & 0 & 0 & 0 \\ 0 & -2t_{11}-t_{22}+\sigma & 0 & 0 \\ 0 & 0 & t_{22}+\sigma & 0 \\ 0 & 0 & 0 & t_{22}+\sigma \end{pmatrix}. \tag{3.62}$$

To have multi channel dragons, namely to satisfy the equation Eq. (3.6), set

$$\begin{pmatrix} 2t_1-2t_2+2t_3-t_4+\epsilon & 0 & 0 & 0 \\ 0 & -2t_1-2t_2-2t_3-t_4+\epsilon & 0 & 0 \\ 0 & 0 & 2t_2-t_4+\epsilon & 0 \\ 0 & 0 & 0 & 2t_2-t_4+\epsilon \end{pmatrix} = \begin{pmatrix} 2t_{11}-t_{22}+\sigma & 0 & 0 & 0 \\ 0 & -2t_{11}-t_{22}+\sigma & 0 & 0 \\ 0 & 0 & t_{22}+\sigma & 0 \\ 0 & 0 & 0 & t_{22}+\sigma \end{pmatrix}. \tag{3.63}$$

This gives

$$\begin{aligned} 2t_1-2t_2+2t_3-t_4+\epsilon &= 2t_{11}-t_{22}+\sigma \\ -2t_1-2t_2-2t_3-t_4+\epsilon &= -2t_{11}-t_{22}+\sigma \\ 2t_2-t_4+\epsilon &= t_{22}+\sigma \\ 2t_2-t_4+\epsilon &= t_{22}+\sigma \end{aligned}. \tag{3.64}$$

Solve these equations

$$
\begin{aligned}
t_{11} &= t_1 + t_3 \\
t_{22} &= 2t_2 \qquad . \\
\sigma &= -t_4 + \epsilon
\end{aligned}
\tag{3.65}
$$

Therefore, if we choose the lead matrix elements as the solutions in Eq. (3.65), and choose the mapping matrix to be $\mathbf{X}$, the mapping equation Eq. (3.7) is satisfied. The mapping matrix $\mathbf{X}$ and its transpose can be written in terms of eigenvectors of the permutation matrix

$$\mathbf{X} = \mathbf{X_{new}} \mathbf{X_{map}} \,. \tag{3.66}$$

$$\mathbf{X_{new}} = \begin{pmatrix} \mathbf{X_{block}} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{pmatrix} . \tag{3.67}$$

$$\mathbf{X_{block}} = \begin{pmatrix} \mathbf{V_1^4} & \mathbf{V_2^4} & \mathbf{V_3^4} & \mathbf{V_4^4} \end{pmatrix} = \begin{pmatrix} -\frac{1}{2} & \frac{1}{2} & 0 & -\frac{1}{\sqrt{2}} \\ \frac{1}{2} & \frac{1}{2} & -\frac{1}{\sqrt{2}} & 0 \\ -\frac{1}{2} & \frac{1}{2} & 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{\sqrt{2}} & 0 \end{pmatrix} . \tag{3.68}$$

$$\mathbf{X} = \begin{pmatrix} \begin{pmatrix} \mathbf{V_1^4} & \mathbf{V_2^4} & \mathbf{V_3^4} & \mathbf{V_4^4} \end{pmatrix} & \mathbf{0} \\ \mathbf{0} & \mathbf{I_{4\times 4}} \end{pmatrix} \begin{pmatrix} \mathbf{V_1^{8\dagger}} \\ \mathbf{V_2^{8\dagger}} \\ \mathbf{V_3^{8\dagger}} \\ \mathbf{V_4^{8\dagger}} \\ \mathbf{V_5^{8\dagger}} \\ \mathbf{V_6^{8\dagger}} \\ \mathbf{V_7^{8\dagger}} \\ \mathbf{V_8^{8\dagger}} \end{pmatrix} . \tag{3.69}$$

$$\mathbf{X}^\dagger = \begin{pmatrix} \mathbf{V_1^8} & \mathbf{V_2^8} & \mathbf{V_3^8} & \mathbf{V_4^8} & \mathbf{V_5^8} & \mathbf{V_6^8} & \mathbf{V_7^8} & \mathbf{V_8^8} \end{pmatrix} \begin{pmatrix} \begin{pmatrix} \mathbf{V_1^{4\dagger}} \\ \mathbf{V_2^{4\dagger}} \\ \mathbf{V_3^{4\dagger}} \\ \mathbf{V_4^{4\dagger}} \end{pmatrix} & \mathbf{0} \\ \mathbf{0} & \mathbf{I_{4\times 4}} \end{pmatrix} . \tag{3.70}$$

Assuming that $\mathbf{W}$ has the following form

$$\mathbf{W} = \begin{pmatrix} b_{11}\mathbf{V_1^{8\dagger}} + b_{12}\mathbf{V_2^{8\dagger}} + b_{13}\mathbf{V_3^{8\dagger}} + b_{14}\mathbf{V_4^{8\dagger}} \\ b_{21}\mathbf{V_1^{8\dagger}} + b_{22}\mathbf{V_2^{8\dagger}} + b_{23}\mathbf{V_3^{8\dagger}} + b_{24}\mathbf{V_4^{8\dagger}} \\ b_{31}\mathbf{V_1^{8\dagger}} + b_{32}\mathbf{V_2^{8\dagger}} + b_{33}\mathbf{V_3^{8\dagger}} + b_{34}\mathbf{V_4^{8\dagger}} \\ b_{41}\mathbf{V_1^{8\dagger}} + b_{42}\mathbf{V_2^{8\dagger}} + b_{43}\mathbf{V_3^{8\dagger}} + b_{44}\mathbf{V_4^{8\dagger}} \end{pmatrix} . \tag{3.71}$$

For mapping equation Eq. (3.6)

$$\mathbf{W}\mathbf{X}^{\dagger} = \begin{pmatrix} b_{11} & b_{12} & b_{13} & b_{14} & 0 & 0 & 0 & 0 \\ b_{21} & b_{22} & b_{23} & b_{24} & 0 & 0 & 0 & 0 \\ b_{31} & b_{32} & b_{33} & b_{34} & 0 & 0 & 0 & 0 \\ b_{41} & b_{42} & b_{43} & b_{44} & 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \begin{pmatrix} \mathbf{V_1^{4\dagger}} \\ \mathbf{V_2^{4\dagger}} \\ \mathbf{V_3^{4\dagger}} \\ \mathbf{V_4^{4\dagger}} \end{pmatrix} & \mathbf{0} \\ \mathbf{0} & \mathbf{I_{4\times 4}} \end{pmatrix} . \tag{3.72}$$

Rewrite

$$\mathbf{W}\mathbf{X}^{\dagger} = \begin{pmatrix} \mathbf{B_{parameter}} & \mathbf{0} \end{pmatrix} \begin{pmatrix} \begin{pmatrix} \mathbf{V_1^{4\dagger}} \\ \mathbf{V_2^{4\dagger}} \\ \mathbf{V_3^{4\dagger}} \\ \mathbf{V_4^{4\dagger}} \end{pmatrix} & \mathbf{0} \\ \mathbf{0} & \mathbf{I_{4\times 4}} \end{pmatrix} . \tag{3.73}$$

Here

$$\mathbf{B_{parameter}} = \begin{pmatrix} b_{11} & b_{12} & b_{13} & b_{14} \\ b_{21} & b_{22} & b_{23} & b_{24} \\ b_{31} & b_{32} & b_{33} & b_{34} \\ b_{41} & b_{42} & b_{43} & b_{44} \end{pmatrix} . \tag{3.74}$$

So Eq. (3.72) becomes

$$\mathbf{W}\mathbf{X}^{\dagger} = \begin{pmatrix} \mathbf{B_{parameter}}\mathbf{X^{\dagger}_{block}} & \mathbf{0} \end{pmatrix} . \tag{3.75}$$

To satisfy the mapping equation Eq. (3.6),

$$\mathbf{B_{parameter}}\mathbf{X^{\dagger}_{block}} = \mathbf{I} . \tag{3.76}$$

Since $\mathbf{X_{block}}$is a unitary matrix

$$\mathbf{B_{parameter}} = \mathbf{X_{block}} \, . \tag{3.77}$$

So $\mathbf{W}$ can be written as

$$\mathbf{W} = \mathbf{X_{block}} \begin{pmatrix} \mathbf{V_1^{8\dagger}} \\ \mathbf{V_2^{8\dagger}} \\ \mathbf{V_3^{8\dagger}} \\ \mathbf{V_4^{8\dagger}} \end{pmatrix} \, . \tag{3.78}$$

$\mathbf{W}$ should be a non-negative matrix, therefore the orders of the eigenvectors in the $\mathbf{X_{block}}$ and the 4 eigenvectors in $\mathbf{X_{map}}$ should be chosen carefully. The order of the eigenvectors as rows in $\mathbf{X_{map}}$ also determine the relationships between lead matrix elements and blob matrix elements in Eq. (3.65).

Using Eq. (3.78)

$$\mathbf{W} = \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & 0 & 0 & \frac{1}{\sqrt{2}} & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & 0 & 0 & \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & 0 & 0 & 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & \frac{1}{\sqrt{2}} & 0 & 0 & 0 & \frac{1}{\sqrt{2}} \end{pmatrix} \, . \tag{3.79}$$

As in the last section, the mapping equation Eq. (3.8) is automatically satisfied.

Thus multi-channel quantum dragons have been found in a 8 atoms per slice rectangular blob connected to 4 atoms per slice rectangular leads. As in the last subsection, the parameters still need to be tuned so that more than one channel can be opened simultaneously. The eigen equation to solve for the energy ranges for each mode is

$$[-\mathbf{B}_L^T e^{-iq} + (\mathbf{A}_L - E\mathbf{I}) - \mathbf{B}_L e^{iq}]\vec{\phi}_j = \lambda_j(E,q)\vec{\phi}_j \tag{3.80}$$

with

$$\lambda_j(E,q) = 0\,. \tag{3.81}$$

Substitute the $\mathbf{A}_L$ and $\mathbf{B}_L$ into Eq. (3.36) to give

$$[\epsilon\mathbf{I} - t_{11}\mathbf{P}^1 - t_{11}\mathbf{P}^{-1} - t_{22}\mathbf{P}^2 - E\mathbf{I} - 2\cos q\mathbf{I}]\vec{\phi}_j = \lambda_j(E,q)\vec{\phi}_j\,. \tag{3.82}$$

The eigenvalues of a $m_L \times m_L$ permutation matrix $\mathbf{P}^1$ are

$$e^{2\pi i(j-1)/m_L} \tag{3.83}$$

where $j = 1, 2, \cdots, m_L$.

Therefore the 4 eigenvalues of Eq. (3.82) are

$$\lambda_j = \sigma - E - 2\cos q_j - 2t_{11}\cos\frac{\pi(j-1)}{2} - t_{22}e^{(j-1)\pi i} \tag{3.84}$$

where $j = 1, 2, 3, 4$.

Set these eigenvalues to zero, solve for $\cos q_j$, to give

$$\begin{aligned}
\cos q_1 &= \frac{1}{2}(\sigma - E - 2t_{11} - t_{22}) \\
\cos q_2 &= \frac{1}{2}(\sigma - E + t_{22}) \\
\cos q_3 &= \frac{1}{2}(\sigma - E + 2t_{11} - t_{22}) \\
\cos q_4 &= \frac{1}{2}(\sigma - E + t_{22})
\end{aligned}\,. \tag{3.85}$$

Since $-1 \leq \cos q \leq 1$, the energy ranges for each channel are

$$\begin{aligned}
\sigma - 2 - 2t_{11} - t_{22} \leq & E \leq \sigma + 2 - 2t_{11} - t_{22} \\
\sigma - 2 + t_{22} \leq & E \leq \sigma + 2 + t_{22} \\
\sigma - 2 + 2t_{11} - 2t_{22} \leq & E \leq \sigma + 2 + 2t_{11} \\
\sigma - 2 + t_{22} \leq & E \leq \sigma + 2 + t_{22}
\end{aligned}\,. \tag{3.86}$$

To open more than 4 channels simultaneously, set

$$\begin{aligned} \sigma - 2 + t_{22} &< \sigma + 2 - 2t_{11} - t_{22} \\ \sigma - 2 + 2t_{11} - t_{22} &< \sigma + 2 - 2t_{11} - t_{22} \end{aligned} \tag{3.87}$$

to give

$$\begin{aligned} t_{11} + t_{22} &< 2 \\ t_{11} &< 1 \end{aligned} . \tag{3.88}$$

To validate the result obtained in this subsection, the matrix method is used to calculate the transmission of a structure. The structure consists of a rectangular blob connected to rectangular leads. There are 4 slices in the blob and in each slice there are 8 atoms. There are 4 atoms in each lead slice. The $\mathbf{A}_l$, $\mathbf{A}_L$, $\mathbf{B}_l$, $\mathbf{B}_L$ and $\mathbf{W}$ in this structure are chosen to be the same as stated in Eq. (3.43) -Eq. (3.46) and Eq. (3.79). Also Eq. (3.65) is satisfied. Furthermore, parameters are tuned to satisfy Eq. (3.88) to show 4 open channels.

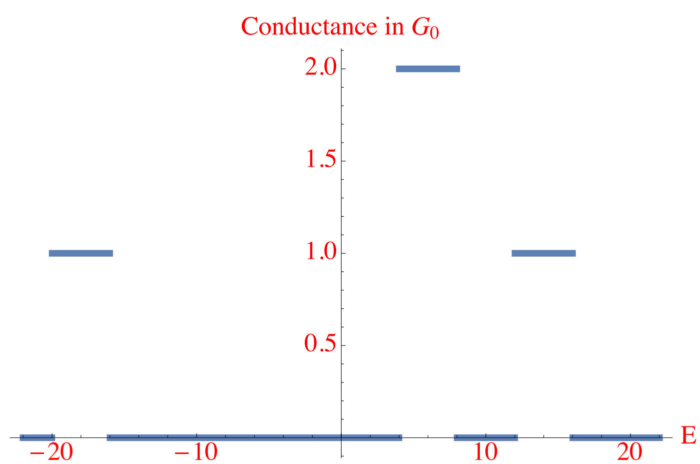

Figure 3.13: Conductance from 4:8:4 quantum dragons: 2 open channels case[13]

[13]The diagram shows a multi-channel quantum dragon from a 8 atoms per slice rectangular nanotube blob connected to 4 atoms per slice rectangular nanotube leads. The transmission for each channel is calculated

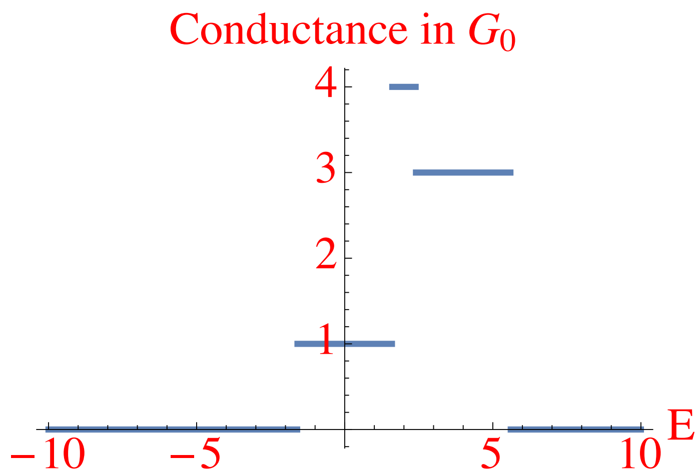

Figure 3.14: Conductance from 4:8:4 quantum dragons: 4 open channels case[14]

3.2.1 General method to find multi-channel quantum dragons in rectangular nanotubes

In this subsection, the method for finding multi-channel quantum dragons in generic rectangular nanotubes is shown.

Assume there are m_l atoms in a slice of the blob, the intra-slice matrix associated with the blob is

$$\mathbf{A}_l = \begin{cases} \epsilon\mathbf{I} - \sum_{k=1}^{\frac{m_l-1}{2}} t_k(\mathbf{P}^k + \mathbf{P}^{-k}), & \text{for } m_l \text{ odd} \\ \epsilon\mathbf{I} - \sum_{k=1}^{\frac{m_l}{2}-1} t_k(\mathbf{P}^k + \mathbf{P}^{-k}) - t_{\frac{m_l}{2}}\mathbf{P}^{\frac{m_l}{2}}, & \text{for } m_l \text{ even} \end{cases} . \tag{3.89}$$

from the matrix method. There are 4 slices in the blob. It can be seen that two channels have same energy ranges. The matrix parameters have been set as follows: $\epsilon = 3$, $t_1 = 3$, $t_2 = 2$, $t_3 = 5$ and $t_4 = 1$, which gives $\sigma = 2$, $t_{11} = 8$ and $t_{22} = 4$.

[14]The diagram shows a multi-channel quantum dragon from a 8 atoms per slice rectangular nanotube blob connected to 4 atoms per slice rectangular nanotube leads. The transmission for each channel is calculated from the matrix method. There are 4 slices in the blob when set into the matrix. It can be seen that the 4 channels share some energy ranges. The matrix parameters have been set as follows: $\epsilon = 3$, $t_1 = 0.5$, $t_2 = 0.3$,$t_3 = 0.3$ and $t_4 = 0.2$, which gives $\sigma = 2.8$, $t_{11} = 0.8$ and $t_{22} = 0.8$.

The eigenvalues of the matrix $\mathbf{A}_l$ are

$$\lambda_j = \begin{cases} \epsilon - \sum_{k=1}^{\frac{m_l-1}{2}} 2t_k \cos\left(\frac{2\pi(j-1)}{m_l}\right)^k, & \text{for } m_l \text{ odd} \\ \epsilon - \sum_{k=1}^{\frac{m_l}{2}-1} 2t_k \cos\left(\frac{2\pi(j-1)}{m_l}\right)^k - t_{\frac{m_l}{2}} e^{(j-1)\pi}, & \text{for } m_l \text{ even} \end{cases} . \tag{3.90}$$

Here $j = 1, 2, 3 \cdots, m_l$.

The eigenvectors of the matrix $\mathbf{A}_l$ are

$$v_j = \frac{1}{\sqrt{m_l}} \begin{pmatrix} e^{\frac{2(j-1)\pi*0}{m_l}} & e^{\frac{2(j-1)\pi*1}{m_l}} & \cdots & e^{\frac{2(j-1)\pi*(m_l-1)}{m_l}} \end{pmatrix}^T , \tag{3.91}$$

where $j = 1, 2, 3 \cdots, m_l$.

Since the eigenvalues are real, $v_j + v_j^*$ are also eigenvectors of $\mathbf{A}_l$. Introduce real eigenvectors

$$\mathbf{V}_j^{m_l} = \frac{v_j + v_j^*}{\sqrt{2}} = \sqrt{\frac{2}{m_l}} \begin{pmatrix} \cos\frac{2(j-1)\pi*0}{m_l} & \cos\frac{2(j-1)\pi*1}{m_l} & \cdots & \cos\frac{2(j-1)\pi*(m_l-1)}{m_l} \end{pmatrix}^T . \tag{3.92}$$

Here j indicates the j's eigenvectors and m_l in the superscript indicates the dimension of the eigenvectors.

Introduce $\mathbf{X}_{map}$

$$\mathbf{X}_{map} = \begin{pmatrix} \mathbf{V}_1^{m_l\dagger} \\ \mathbf{V}_2^{m_l\dagger} \\ \vdots \\ \mathbf{V}_{m_l}^{m_l\dagger} \end{pmatrix} . \tag{3.93}$$

Since $\mathbf{X}_{map}$ is unitary, $\mathbf{A}_l$ can be diagonalized as

$$\mathbf{X}_{map} \mathbf{A}_l \mathbf{X}_{map}^\dagger = \mathbf{A}_{diagonal} . \tag{3.94}$$

here $\mathbf{A}_{diagonal}$ is

$$\mathbf{A}_{diagonal} = \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 & 0 \\ 0 & \lambda_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & \lambda_{m_l-1} & 0 \\ 0 & 0 & \cdots & 0 & \lambda_{m_l} \end{pmatrix} . \tag{3.95}$$

Introduce the transformation matrix $\mathbf{X}$

$$\mathbf{X} = \mathbf{X}_{new}\mathbf{X}_{map} , \tag{3.96}$$

where $\mathbf{X}_{new}$ is a block matrix

$$\mathbf{X}_{new} = \begin{pmatrix} \mathbf{X}_{block} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{pmatrix} . \tag{3.97}$$

A successful mapping is defined as

$$\mathbf{X}\mathbf{A}\mathbf{X}^{\dagger} = \begin{pmatrix} \tilde{\mathbf{A}} & \mathbf{0} \\ \mathbf{0} & \hat{\mathbf{A}} \end{pmatrix} . \tag{3.98}$$

To have multi-channel quantum dragons, the first equation to be satisfied is

$$\tilde{\mathbf{A}} = \mathbf{A}_L . \tag{3.99}$$

Then the equation becomes

$$\mathbf{X}_{new}\mathbf{X}_{map}\mathbf{A}_l\mathbf{X}_{map}^{\dagger}\mathbf{X}_{new}^{\dagger} = \begin{pmatrix} \mathbf{A}_L & \mathbf{0} \\ \mathbf{0} & \hat{\mathbf{A}} \end{pmatrix} . \tag{3.100}$$

$$\mathbf{X}_{new}\mathbf{A}_{diagonal}\mathbf{X}_{new}^{\dagger} = \begin{pmatrix} \mathbf{A}_L & \mathbf{0} \\ \mathbf{0} & \hat{\mathbf{A}} \end{pmatrix} . \tag{3.101}$$

$$\mathbf{A}_{diagonal} = \mathbf{X}_{new}^{\dagger} \begin{pmatrix} \mathbf{A}_L & \mathbf{0} \\ \mathbf{0} & \hat{\mathbf{A}} \end{pmatrix} \mathbf{X}_{new} \,. \tag{3.102}$$

$$\mathbf{A}_{diagonal} = \begin{pmatrix} \mathbf{X}_{block}^{\dagger} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{pmatrix} \begin{pmatrix} \mathbf{A}_L & \mathbf{0} \\ \mathbf{0} & \hat{\mathbf{A}} \end{pmatrix} \begin{pmatrix} \mathbf{X}_{block} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{pmatrix} \,. \tag{3.103}$$

$$\mathbf{A}_{diagonal} = \begin{pmatrix} \mathbf{X}_{block}^{\dagger}\mathbf{A}_L\mathbf{X}_{block} & \mathbf{0} \\ \mathbf{0} & \hat{\mathbf{A}} \end{pmatrix} \,. \tag{3.104}$$

Since the leads are also rectangular nanotubes, the intra-slice matrix of leads can also be written as Eq.(3.89)

$$\mathbf{A}_L = \begin{cases} \epsilon_{Lead}\mathbf{I} - \sum_{k=1}^{\frac{m_L-1}{2}} t_{kLead}(\mathbf{P}^k + \mathbf{P}^{-k}), & \text{for } m_L \text{ odd} \\ \epsilon_{Lead}\mathbf{I} - \sum_{k=1}^{\frac{m_L}{2}-1} t_{kLead}(\mathbf{P}^k + \mathbf{P}^{-k}) - t_{\frac{m_L}{2}Lead}\mathbf{P}^{\frac{m_L}{2}}, & \text{for } m_L \text{ even} \end{cases} \,. \tag{3.105}$$

here m_L is the number of atoms in a slice of the lead. It can be seen from Eq.(3.104) that $m_l > m_L$.

$\mathbf{A}_L$ can also be diagonalized by the eigenvectors similar to that in Eq.(3.92) but with different dimension m_L

$$\mathbf{V}_j^{m_L} = \frac{v_j + v_j^*}{\sqrt{2}} = \sqrt{\frac{2}{m_L}} \begin{pmatrix} \cos\frac{2(j-1)\pi*0}{m_L} & \cos\frac{2(j-1)\pi*1}{m_L} & \cdots & \cos\frac{2(j-1)\pi*(m_L-1)}{m_L} \end{pmatrix}^T \,. \tag{3.106}$$

$$\mathbf{X}_{block}^{\dagger}\mathbf{A}_L\mathbf{X}_{block} = \mathbf{A}_{Ldiagonal} \,. \tag{3.107}$$

where $\mathbf{X}_{block}^{\dagger}$ is

$$\mathbf{X}_{block}^{\dagger} = \begin{pmatrix} \mathbf{V}_1^{m_L \dagger} \\ \mathbf{V}_2^{m_L \dagger} \\ \vdots \\ \mathbf{V}_{m_L}^{m_L \dagger} \end{pmatrix} \tag{3.108}$$

and $\mathbf{A}_{Ldiagonal}$ is

$$\mathbf{A}_{Ldiagonal} = \begin{pmatrix} \lambda_{Lead1} & 0 & \cdots & 0 & 0 \\ 0 & \lambda_{Lead2} & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & \lambda_{Leadm_L-1} & 0 \\ 0 & 0 & \cdots & 0 & \lambda_{LeadmL} \end{pmatrix} \tag{3.109}$$

with

$$\lambda_{Leadj} = \begin{cases} \epsilon_{Lead} - \sum_{k=1}^{\frac{m_L-1}{2}} 2t_{kLead} \cos\left(\frac{2\pi(j-1)}{m_L}\right)^k, & \text{for } m_L \text{ odd} \\ \epsilon_{Lead} - \sum_{k=1}^{\frac{m_L}{2}-1} 2t_{kLead} \cos\left(\frac{2\pi(j-1)}{m_L}\right)^k - t_{\frac{m_L}{2}Lead} e^{(j-1)\pi}, & \text{for } m_L \text{ even} \end{cases} . \tag{3.110}$$

here $j = 1, 2, 3 \cdots, m_L$.

To satisfy Eq.(3.104)

$$\lambda_j = \lambda_{Leadj} . \tag{3.111}$$

Where $j = 1, 2, 3 \cdots, m_L$.

Therefore provided one uses the $\mathbf{X}$ in Eq. (3.96) and Eq. (3.111), the first mapping equation from equation set Eq. (3.6) to Eq. (3.8)is satisfied. Now move to the second mapping equation.

A successful mapping of the lead-blob connection is defined as

$$\mathbf{W}\mathbf{X}^{\dagger} = \begin{pmatrix} \tilde{\mathbf{W}} & \mathbf{0} \end{pmatrix} . \tag{3.112}$$

From Eq. (3.96), $\mathbf{X}^{\dagger}$ is

$$\mathbf{X}^{\dagger} = \begin{pmatrix} \mathbf{V}_1^{m_l\dagger} & \mathbf{V}_2^{m_l\dagger} & \dots & \mathbf{V}_{m_l}^{m_l\dagger} \end{pmatrix} \begin{pmatrix} \begin{pmatrix} \mathbf{V}_1^{m_L\dagger} \\ \mathbf{V}_2^{m_L\dagger} \\ \vdots \\ \mathbf{V}_{m_L}^{m_L\dagger} \end{pmatrix} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{pmatrix} . \tag{3.113}$$

Assume that $\mathbf{W}$ has the following form

$$\mathbf{W} = \begin{pmatrix} b_{11}\mathbf{V}_1^{m_l\dagger} + b_{12}\mathbf{V}_2^{m_l\dagger} + \cdots + b_{1m_L}\mathbf{V}_{m_L}^{m_l\dagger} \\ b_{21}\mathbf{V}_1^{m_l\dagger} + b_{22}\mathbf{V}_2^{m_l\dagger} + \cdots + b_{2m_L}\mathbf{V}_{m_L}^{m_l\dagger} \\ \vdots \\ b_{m_L1}\mathbf{V}_1^{m_l\dagger} + b_{m_l2}\mathbf{V}_2^{m_l\dagger} + \cdots + b_{m_Lm_L}\mathbf{V}_{m_L}^{m_l\dagger} \end{pmatrix} . \tag{3.114}$$

Then $\mathbf{W}\mathbf{X}^{\dagger}$ is

$$\mathbf{W}\mathbf{X}^{\dagger} = \begin{pmatrix} b_{11} & b_{12} & \cdots & b_{1m_L} & 0 & 0 & \cdots & 0 & 0 \\ b_{11} & b_{12} & \cdots & b_{1m_L} & 0 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ b_{m_L1} & b_{m_L2} & \cdots & b_{m_Lm_L} & 0 & 0 & \cdots & 0 & 0 \end{pmatrix} \begin{pmatrix} \begin{pmatrix} \mathbf{V}_1^{m_L\dagger} \\ \mathbf{V}_2^{m_L\dagger} \\ \vdots \\ \mathbf{V}_{m_L}^{m_L\dagger} \end{pmatrix} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{pmatrix} . \tag{3.115}$$

Let

$$\mathbf{B}_{parameter} = \begin{pmatrix} b_{11} & b_{12} & \cdots & b_{1m_L} \\ b_{11} & b_{12} & \cdots & b_{1m_L} \\ \vdots & \vdots & \ddots & \vdots \\ b_{m_L1} & b_{m_L2} & \cdots & b_{m_Lm_L} \end{pmatrix} . \tag{3.116}$$

And recall that

$$\mathbf{X}^{\dagger}_{block} = \begin{pmatrix} \mathbf{V}^{m_L\dagger}_{1} \\ \mathbf{V}^{m_L\dagger}_{2} \\ \vdots \\ \mathbf{V}^{m_L\dagger}_{m_L} \end{pmatrix} . \tag{3.117}$$

Then

$$\mathbf{W}\mathbf{X}^{\dagger} = \begin{pmatrix} \mathbf{B}_{parameter}\mathbf{X}^{\dagger}_{block} & \mathbf{0} \end{pmatrix} . \tag{3.118}$$

where $\tilde{\mathbf{W}} = \mathbf{B}_{parameter}\mathbf{X}^{\dagger}_{block}$.

The blob will become a multi-channel quantum dragon when $\tilde{\mathbf{W}} = \mathbf{B}_L$. For the rectangular leads that have only nearest-neighbor inter-slice interaction, namely $\mathbf{B}_L = \mathbf{I}$, $\mathbf{B}_{parameter}$ can be solved as

$$\mathbf{B}_{parameter} = \mathbf{X}_{block} . \tag{3.119}$$

Therefore $\mathbf{W}$ is

$$\mathbf{W} = \mathbf{X}_{block} \begin{pmatrix} \mathbf{V}^{m_l\dagger}_{1} \\ \mathbf{V}^{m_l\dagger}_{2} \\ \vdots \\ \mathbf{V}^{m_l\dagger}_{m_L} \end{pmatrix} . \tag{3.120}$$

Since the hopping parameters in $\mathbf{W}$ come from the kinetic energy term of the time-independent Schrödinger equation, $\mathbf{W}$ must be a non-negative matrix

$$\mathbf{W} \geq 0 \,. \tag{3.121}$$

The last mapping equation to be solved is the mapping of the blob inter-slice hopping terms. For the rectangular leads and blob that have only nearest-neighbor inter-slice interaction, the mapping equation is automatically satisfied providing that $\mathbf{X}$ in Eq. (3.96).

$$\mathbf{X}\mathbf{B}_l\mathbf{X}^\dagger = \mathbf{I} = \begin{pmatrix} \mathbf{B}_L & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{pmatrix} \,. \tag{3.122}$$

Where $\mathbf{B}_l$ and $\mathbf{B}_L$ are identity matrices.

To have multi-channel quantum dragons, not only the mapping equations need to be satisfied, but also the propagating mode needs to exist in the lead. In the following subsection, how to find the lead for rectangular nanotube multi-channel quantum dragons is shown.

Assume a lead intra-slice $\mathbf{A}_L$ and inter-slice $\mathbf{B}_L$ interaction are of the following form

$$\mathbf{A}_L = \begin{cases} \epsilon_{Lead}\mathbf{I} - \sum_{k=1}^{\frac{m_L-1}{2}} t_{kLead}(\mathbf{P}^k + \mathbf{P}^{-k}), & \text{for } m_L \text{ odd} \\ \epsilon_{Lead}\mathbf{I} - \sum_{k=1}^{\frac{m_L}{2}-1} t_{kLead}(\mathbf{P}^k + \mathbf{P}^{-k}) - t_{\frac{m_L}{2}Lead}\mathbf{P}^{\frac{m_L}{2}}, & \text{for } m_L \text{ even} \end{cases} \tag{3.123}$$

$$\mathbf{B}_L = t_0\mathbf{I} \,. \tag{3.124}$$

The eigen equation to solve for the lead slice wavefunction is

$$[-\mathbf{B}_L^T e^{-iq} + (\mathbf{A}_L - E\mathbf{I}) - \mathbf{B}_L e^{iq}]\vec{\phi}_j = \lambda_j(E,q)\vec{\phi}_j \,. \tag{3.125}$$

Since $\mathbf{B}_L = t_0\mathbf{I}$, the eigen equation can be written as

$$[\mathbf{A}_L - E\mathbf{I} - 2t_0 \cos q_j \mathbf{I}]\vec{\phi}_j = \lambda_j(E, q)\vec{\phi}_j \, . \tag{3.126}$$

From Eq. (3.110) , the eigenvalues $\lambda_j(E, q)$ in Eq. (3.126) are

For m_L odd

$$\epsilon_{Lead} - E - 2t_0 \cos q_j - \sum_{k=1}^{\frac{m_L-1}{2}} 2t_{kLead} \cos (\frac{2\pi(j-1)}{m_L})^k$$

For m_L even

$$\epsilon_{Lead} - E - 2t_0 \cos q_j - \sum_{k=1}^{\frac{m_L}{2}-1} 2t_{kLead} \cos (\frac{2\pi(j-1)}{m_L})^k - t_{\frac{m_L}{2}Lead} e^{(j-1)\pi} \tag{3.127}$$

Set $\lambda_j(E, q) = 0$

For m_L odd

$$\cos q_j = \frac{1}{2t_0}[\epsilon_{Lead} - E - \sum_{k=1}^{\frac{m_L-1}{2}} 2t_{kLead} \cos (\frac{2\pi(j-1)}{m_L})^k]$$

For m_L even

$$\cos q_j = \frac{1}{2t_0}[\epsilon_{Lead} - E - \sum_{k=1}^{\frac{m_L}{2}-1} 2t_{kLead} \cos (\frac{2\pi(j-1)}{m_L})^k - t_{\frac{m_L}{2}Lead} e^{(j-1)\pi}] \tag{3.128}$$

The energy range of each mode can be solved by setting $-1 \leq \cos q \leq 1$ in Eq. (3.128).

For m_L odd

$$E \geq \epsilon_{Lead} - 2t_0 - \sum_{k=1}^{\frac{m_L-1}{2}} 2t_{kLead} \cos (\frac{2\pi(j-1)}{m_L})^k$$
$$E \leq \epsilon_{Lead} + 2t_0 - \sum_{k=1}^{\frac{m_L-1}{2}} 2t_{kLead} \cos (\frac{2\pi(j-1)}{m_L})^k \tag{3.129}$$

For m_L even

$$\begin{aligned} E &\geq \epsilon_{Lead} - 2t_0 - \sum_{k=1}^{\frac{m_L}{2}-1} 2t_{kLead} \cos\left(\frac{2\pi(j-1)}{m_L}\right)^k - t_{\frac{m_L}{2}Lead} e^{(j-1)\pi} \\ E &\leq \epsilon_{Lead} + 2t_0 - \sum_{k=1}^{\frac{m_L}{2}-1} 2t_{kLead} \cos\left(\frac{2\pi(j-1)}{m_L}\right)^k - t_{\frac{m_L}{2}Lead} e^{(j-1)\pi} \end{aligned} \tag{3.130}$$

To open more than one channel simultaneously, parameters need to be tuned from Eq. (3.129) and Eq. (3.130) so that energy ranges from different modes can have a common part.

CHAPTER 4

CONCLUSIONS

The procedure to use the matrix method to find multi-channel quantum dragons in rectangular nanotubes has been shown. A multi-channel quantum dragon is a nanodevice that may have disorder, but when connected to input and output leads , electrons impinging into it can propagate through with probability 1 in more than one channel. In a two-terminal measurement, the electrical conductance of a multi-channel quantum dragon is the product of number of open channels $m$and the conductance quantum G_0, namely mG_0.This is also the first time the matrix method has been modified to take into account more than one channel in the lead slices. The modification may allow for more realistic nanostructure calculation since practical nanodevices are not idea 1D atom chain.

Multi-channel quantum dragons have been shown in rectangular nanotubes in this thesis. The conductance of a rectangular nanotube multi-channel quantum dragon nanodevice can be as high as $\mathcal{M}G_0$, where $\mathcal{M}$ is the number of atoms in each slice of the lead and G_0 is the conductance quantum. The highest conductance happens as all the channels are open at the same time.

No experimental realization of rectangular nanotubes has been reported yet. Nevertheless, single-atom-thick Fe layer with a square lattice structure has been report recently[18].

It is expected that in the future, rectangular nanotubes can be made from this kind of single-atom-thick square lattices, which may make application of rectangular nanotube multi-channel quantum dragons possible.

Beside rectangular nanotubes, there are other types of nanostructures such as zigzag single-walled carbon nanotubes (SWCNTS), armchair SWCNTS and Bethe lattices can form single-channel quantum dragons[16]. Carnon nanotubes are strong candidates for possible novel nanoelectrinic applications[4][3][17][1]. Since electrons can propagate multi-channel quantum dragons with total transmission, multi-channel quantum dragons have potential for some of the same applications as do ballistic electron propagation devices [13][11]. Therefore, finding multi-channel quantum dragons from these structures will be the next stage of this multi-channel quantum dragon study.

Rectangular nanotube multi-channel quantum dragons are examples of linear form quantum dragons in which the nanodevice consists of slices and interactions only between nearest neighbor slices. The future directions of the work therefore also may include research about more complex nanostructures, which include next-nearest neighbor slice hopping terms.

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APPENDIX A

MATRIX METHOD FOR ELECTRON TRANSMISSION CALCULATION AND SINGLE-CHANNEL QUANTUM DRAGONS

A.1 Matrix method for solving quantum transmission problem

In this appendix, matrix method and its application in calculation of transmission from single channel quantum dragons have been reviewed briefly.

A.1.1 Method of finite differences

In lots of practical problems, the Schrödinger equation can not been solved analytically. Therefore these problems require a numerical solution. The most widely used way to obtain a numerical solution for the Schrödinger equation is converting the differential equation to a matrix equation. Using the 1D case as an example, the following part shows how this is done.

Firstly, we represent the wavefucntion $\Psi(x,t)$ by a column vector $\{\psi_1(t)\ \psi_2(t)\cdots\}^T$ containing its values around each of the lattice points at time t. The spatial lattice is regular, with lattice spacing a.

Next, we obtain the matrix representation of the Hamiltonian operator

$$H_{op} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U(x) \tag{A.1}$$

recall the approximation

$$(\frac{\partial^2\Psi}{\partial x^2})_{x=x_n} \approx \frac{1}{a^2}\left(\Psi(x_n+1) - 2\Psi(x_n) + \Psi(x_n-1)\right) \tag{A.2}$$

and

$$U(x)\Psi(x) = U(x_n)\Psi(x_n)\ . \tag{A.3}$$

The above procedure is called the finite difference method.

Then the Schrödinger equation becomes

$$
\begin{aligned}
i\hbar \frac{d\psi_n}{dt} &= [H_{op}]_{x=x_n} = (U_n + 2t_0)\psi_n - t_0\psi_{n-1} - t_0\psi_{n+1} \\
&= \sum_m [(U_n + 2t_0)\delta_{n,m} - t_0\delta_{n,m+1} - t_0\delta_{n,m-1}]\psi_m
\end{aligned} \tag{A.4}
$$

where $\delta_{n,m}$ is Kronecker delta.

Then the Schrödinger equation can be written as a matrix equation

$$
i\hbar \frac{d}{dt}\vec{\psi}(t) = [\mathbf{H}]\vec{\psi}(t) \tag{A.5}
$$

Where $\psi(t)$ is a column vector

$$
\vec{\psi}(t) = (\psi_1(t)\ \psi_2(t) \cdots)^T \tag{A.6}
$$

and $[\mathbf{H}]$ is a matrix with matrix elements

$$
\mathbf{H}_{n,m} = (U_n + 2t_0)\delta_{n,m} - t_0\delta n, m+1 - t_0\delta n, m-1 \tag{A.7}
$$

with

$$
t_0 = \hbar^2/2ma^2 \tag{A.8}
$$

and

$$
U_n = U(x_n)\ . \tag{A.9}
$$

Now assume that the Hamiltonian is time independent. To solve the matrix equation, the eigenvectors α and associated eigenvalues E_α of $\mathbf{H}$ must be found first

$$
[\mathbf{H}]\vec{\alpha} = E_\alpha\vec{\alpha}\ . \tag{A.10}
$$

It can been shown that the complete form of the solution to the Eq. (5) is

$$
\vec{\psi}(t) = \sum_\alpha C_\alpha e^{-iE_\alpha t/\hbar}\vec{\alpha}\ . \tag{A.11}
$$

The coefficients C_α are time independent and found from the initial condition $\vec{\psi}(0) = \sum_\alpha C_\alpha \vec{\alpha}$.

A.1.2 Matrix method for quantum transmission

Rewrite Eq. (A.10), drop the α for conciseness, to give

$$(\mathbf{H} - E)\vec{\psi} = 0 \, . \tag{A.12}$$

The explicit matrix form of H depends on details of the structure of the leads and of the device. Consider the following 1D discretization diagram

$$\begin{array}{ccccccccccccccccc} \cdots & -t_0 & \rightarrow & (0) & \leftarrow & -w & \rightarrow & (a) & \leftarrow & -t_{12} & \rightarrow & (b) & \leftarrow & -u & \rightarrow & (1) & \leftarrow & -t_0 & \cdots \\ \cdots & & & \epsilon_0 & & & & \epsilon_a & & & & \epsilon_b & & & & \epsilon_0 & & & \cdots \\ \cdots & & & \psi_0 & & & & \psi_a & & & & \psi_b & & & & \psi_1 & & & \cdots \end{array} \, . \tag{A.13}$$

where ψ_i is the wavefunction at each atom site, ϵ's are the onsite energies for different atoms, t's , w and u are hopping terms between nearest atoms.

The infinite matrix Eq. (A.12) then is

$$\begin{pmatrix}
\ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \\
\cdots & K_0 & -t_0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots \\
\cdots & -t_0 & K_0 & -t_0 & 0 & 0 & 0 & 0 & \cdots & \\
\cdots & 0 & -t_0 & K_0 & -w & 0 & 0 & 0 & 0 & \cdots \\
\cdots & 0 & 0 & -w & \epsilon_a - E & -t_{12} & 0 & 0 & 0 & \cdots \\
\cdots & 0 & 0 & 0 & -t_{12} & \epsilon_b - E & -u & 0 & 0 & \cdots \\
\cdots & 0 & 0 & 0 & 0 & -u & K_0 & -t_0 & 0 & \cdots \\
\cdots & 0 & 0 & 0 & 0 & 0 & -t_0 & K_0 & -t_0 & \cdots \\
\cdots & 0 & 0 & 0 & 0 & 0 & 0 & -t_0 & K_0 & \cdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots
\end{pmatrix}
\begin{pmatrix} \vdots \\ \psi_{-2} \\ \psi_{-1} \\ \psi_0 \\ \psi_a \\ \psi_b \\ \psi_{+1} \\ \psi_{+2} \\ \psi_{+3} \\ \vdots \end{pmatrix}
=
\begin{pmatrix} \vdots \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \vdots \end{pmatrix} . \tag{A.14}$$

where $K_0 = \epsilon_0 - E$.

Using the $ansatz$ from [16], the slice wave function of the blob and leads can be written as

$$\psi_n = \begin{cases} e^{iqna} + re^{-iqna} & n \leq 0 \\ \\ t_T e^{iq(n-1)a} & n \geq 1 \end{cases} . \tag{A.15}$$

Substitute the $ansatz$ in the tight-banding equation Eq. (A.14) for the outgoing lead $(n \geq 1)$

$$\begin{aligned} -t_0 t_T e^{i(n-2)qa} + (\epsilon_0 - E)t_T e^{i(n-1)qa} - t_0 t_T e^{inqa} = 0 \\ -t_0 e^{-iqa} + (\epsilon_0 - E) - t_0 e^{iqa} = 0 \\ \epsilon_0 - E = 2t_0 \cos qa \,. \end{aligned} \tag{A.16}$$

Substitute the $ansatz$ in the tight-banding equation Eq. (A.14) for the incoming lead $(n \leq 0)$

$$\begin{aligned} -t_0(e^{iq(n-1)a} + re^{-iq(n-1)a}) + (\epsilon_0 - E)(e^{iqna} + re^{iqna}) - t_0(e^{iq(n+1)a} + re^{iq(n+1)a}) = 0 \\ -t_0 e^{-iqa} - t_0 e^{iqa} + (\epsilon_0 - E) - t_0 re^{-iq(2n-1)a} + (\epsilon_0 - E)re^{-2iqna} - t_0 re^{-iq(2n+1)a} = 0 \\ (-t_0 e^{-iqa} + \epsilon_0 - E - t_0 e^{iqa})(1 + re^{-2iqna}) = 0 \\ (\epsilon_0 - E - 2t_0 cos(qa))(1 + re^{-2iqna}) = 0 \,. \end{aligned} \tag{A.17}$$

this equation can also be satisfied by the last equation in Eq. (A.16).

The four rows of matrix equation that have yet to be satisfied in Eq. (A.14) are

$$\begin{pmatrix} -t_0 & \epsilon_0 - E & -w & 0 & 0 & 0 \\ 0 & -w & \epsilon_a - E & -t_{12} & 0 & 0 \\ 0 & 0 & -t_{12} & \epsilon_b - E & -u & 0 \\ 0 & 0 & 0 & -u & \epsilon_0 - E & -t_0 \end{pmatrix} \begin{pmatrix} \psi_{-1} \\ \psi_0 \\ \psi_a \\ \psi_b \\ \psi_1 \\ \psi_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}. \tag{A.18}$$

Using the *ansatz* again

$$\begin{pmatrix} -t_0 & \epsilon_0 - E & -w & 0 & 0 & 0 \\ 0 & -w & \epsilon_a - E & -t_{12} & 0 & 0 \\ 0 & 0 & -t_{12} & \epsilon_b - E & -u & 0 \\ 0 & 0 & 0 & -u & \epsilon_0 - E & -t_0 \end{pmatrix} \begin{pmatrix} e^{-iqa} + re^{iqa} \\ 1 + r \\ \psi_a \\ \psi_b \\ t_T \\ t_T e^{iqa} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}. \tag{A.19}$$

Multiplying through gives

$$\begin{pmatrix} -t_0 e^{-iqa} - t_0 r e^{iqa} + \epsilon_0 + \epsilon_0 r - E - Er - w\psi_a \\ -w - wr + (\epsilon_a - E)\psi_a - t_{12}\psi_b \\ -t_{12}\psi_a + (\epsilon_b - E)\psi_b - ut_T \\ -u\psi_b + \epsilon_0 t_T - Et_T - t_0 t_T e^{iqa} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}. \tag{A.20}$$

Using $-E = t_0 e^{iqa} + t_0 e^{-iqa} - \epsilon_0$ in Eq. (15) , the bottom equation of equation (19) can be written as

$$\begin{aligned} -u\psi_b + \epsilon_0 t_T - E t_T - t_0 t_T e^{iqa} &= -u\psi_b + t_0(e^{iqa} + e^{-iqa})t_T - t_0 t_T e^{iqa} \\ &= -u\psi_b + t_0 t_T e^{iqa} + t_0 t_T e^{-iqa} - t_0 t_T e^{iqa} \\ &= -u\psi_b + t_0 t_T e^{-iqa}\,. \end{aligned} \tag{A.21}$$

Using $-E = t_0 e^{iqa} + t_0 e^{-iqa} - \epsilon_0$, the top equation of equation (19) can be written as

$$\begin{aligned} -t_0 e^{-iqa} - t_0 r e^{iqa} + \epsilon_0 + \epsilon_0 r - E - Er - w\psi_a &= -t_0 e^{-iqa} - t_0 r e^{iqa} + t_0 e^{iqa} + \\ &\quad t_0 e^{-iqa} + r t_0 e^{iqa} + r t_0 e^{-iqa} - w\psi_a \\ &= t_0 e^{iqa} + r t_0 e^{-iqa} - w\psi_a\,. \end{aligned} \tag{A.22}$$

Eq. (A.19) thus becomes

$$\begin{pmatrix} t_0 e^{iqa} + r t_0 e^{-iqa} - w\psi_a + (t_0 e^{-iqa} - t_0 e^{-iqa}) \\ -w - wr + (\epsilon_a - E)\psi_a - t_{12}\psi_b \\ -t_{12}\psi_a + (\epsilon_b - E)\psi_b - u t_T \\ -u\psi_b + t_0 t_T e^{-iqa} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}. \tag{A.23}$$

which can be written into a matrix equation form

$$\begin{pmatrix} t_0 e^{-iqa} & -w & 0 & 0 \\ -w & \epsilon_a - E & -t_{12} & 0 \\ 0 & -t_{12} & \epsilon_b - E & -u \\ 0 & 0 & -u & t_0 e^{-iqa} \end{pmatrix} \begin{pmatrix} 1 + r \\ \psi_a \\ \psi_b \\ t_T \end{pmatrix} = \begin{pmatrix} -2it_0 \sin qa \\ 0 \\ 0 \\ 0 \end{pmatrix}. \tag{A.24}$$

Solving this matrix equation, the transmission $\mathcal{T}(E)$ can be obtained as $\mathcal{T}(E) = |t_T|^2 = t_T t_T^*$.

The matrix equation used to calculate the transmission can be generalized to non-1D cases. Generally there are three types of sites in the blob: sites directly connected to the input lead, in; sites directly connected to the output lead, ut; sites not directly connected to either the input or output lead, not. Similar to the 1D case, the blob now is arranged into three parts with the different types of sites.

In these general cases, $\mathcal{T}(E)$ is given by the solution of matrix equation

$$\begin{pmatrix} \xi(E) & \vec{w}^{\dagger} & \vec{0}^{\dagger} & \vec{0}^{\dagger} & 0 \\ \vec{w} & \mathbf{A}_{in} - E\mathbf{I} & \mathbf{B}_{in,not} & \mathbf{B}_{in,ut} & \vec{0} \\ \vec{0} & \mathbf{B}^{\dagger}_{in,not} & \mathbf{A}_{not} - E\mathbf{I} & \mathbf{B}_{not,ut} & \vec{0} \\ \vec{0} & \mathbf{B}^{\dagger}_{in,ut} & \mathbf{B}^{\dagger}_{not,ut} & \mathbf{A}_{ut} - E\mathbf{I} & \vec{u} \\ 0 & \vec{0} & \vec{0} & \vec{u}^{\dagger} & \xi(E) \end{pmatrix} \begin{pmatrix} 1+r \\ \vec{\psi}_{in} \\ \vec{\psi}_{not} \\ \vec{\psi}_{ut} \\ t_T \end{pmatrix} = \begin{pmatrix} 2i\mathcal{I}m(\xi) \\ \vec{0} \\ \vec{0} \\ \vec{0} \\ 0 \end{pmatrix} \tag{A.25}$$

where $\xi(E)$ is defined as

$$\xi(E) = t_0 e^{-iqa} \tag{A.26}$$

and $\mathcal{I}m(\xi)$ is the imaginary part of $\xi(E)$.

A.1.3 Linear form blobs and mapping onto a one dimension chain

In principle transmission of any blob can be obtain from the solution of a matrix equation as in Eq. (A.25). Usually this involves taking the inverse of an extremely large matrix, which makes exact solution of the matrix equation in general not possible. Using the technique introduced in [16], a mapping from the original large matrix to a much smaller matrix can make the search for quantum dragons easier.

A linear blob is a blob that is composed of l different slices, and the slice i interacts only with slices $i-1$ and $i+1$ (with $1 \leq i \leq l$). In a linear blob, each slice only has interactions with nearest slices. So the matrix in matrix equation Eq. (A.25) becomes

$$\mathbf{N}_l = \begin{pmatrix} \xi(E) & \vec{w}^\dagger & \vec{0}^\dagger & \vec{0}^\dagger & \cdots & \vec{0}^\dagger & \vec{0}^\dagger & 0 \\ \vec{w} & \mathbf{A}_1 - E\mathbf{I} & \mathbf{B}_{12} & \mathbf{0} & \cdots & \mathbf{0} & \mathbf{0} & \vec{0} \\ \vec{0} & \mathbf{B}_{21} & \mathbf{A}_2 - E\mathbf{I} & \mathbf{B}_{23} & \cdots & \mathbf{0} & \mathbf{0} & \vec{0} \\ \vec{0} & \mathbf{0} & \mathbf{B}_{32} & \mathbf{A}_3 - E\mathbf{I} & & \mathbf{0} & \mathbf{0} & \vec{0} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ \vec{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{A}_{l-1} - E\mathbf{I} & \mathbf{B}_{l-1,l} & \vec{0} \\ \vec{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{B}_{l,l-1} & \mathbf{A}_l - E\mathbf{I} & \vec{u} \\ 0 & \vec{0}^\dagger & \overrightarrow{0}^\dagger & \vec{0}^\dagger & \cdots & \vec{0}^\dagger & \vec{u}^\dagger & \xi(E) \end{pmatrix} . \tag{A.27}$$

Here A_i is a $m_i \times m_i$ matrix containing all the intra-slice couplings and on-site energies. $B_{i,i+1}$ is a $m_i \times m_{i+1}$ matrix containing inter-slice couplings.

Then the matrix equation becomes

$$\mathbf{N}_l \times \begin{pmatrix} 1+r \\ \vec{\psi}_1 \\ \vec{\psi}_2 \\ \vdots \\ \vec{\psi}_{l-1} \\ \vec{\psi}_l \\ t_T \end{pmatrix} = \begin{pmatrix} 2i\mathcal{I}m(\xi) \\ \vec{0} \\ \vec{0} \\ \vdots \\ \vec{0} \\ \vec{0} \\ 0 \end{pmatrix} . \tag{A.28}$$

Introduce the $l \times l$ block-diagonal transformation matrices

$$\hat{\mathbf{X}} = \begin{pmatrix} 1 & & & & & & & \\ & \mathbf{X}_1 & & & & & & \\ & & \mathbf{X}_2 & & & & & \\ & & & \mathbf{X}_3 & & & & \\ & & & & \ddots & & & \\ & & & & & \mathbf{X}_{l-1} & & \\ & & & & & & \mathbf{X}_l & \\ & & & & & & & 1 \end{pmatrix}. \tag{A.29}$$

and

$$\hat{\mathbf{Y}}^\dagger = \begin{pmatrix} 1 & & & & & & & \\ & \mathbf{Y}_1^\dagger & & & & & & \\ & & \mathbf{Y}_2^\dagger & & & & & \\ & & & \mathbf{Y}_3^\dagger & & & & \\ & & & & \ddots & & & \\ & & & & & \mathbf{Y}_{l-1}^\dagger & & \\ & & & & & & \mathbf{Y}_l^\dagger & \\ & & & & & & & 1 \end{pmatrix}. \tag{A.30}$$

In Eq. (A.28), inserting the identity matrix $\mathbf{I} = \hat{Y}^\dagger(\hat{Y}^\dagger)^{-1}$ between the matrix $\mathbf{N}_l$ and the vector gives

$$\hat{\mathbf{X}}\mathbf{N}_l\hat{\mathbf{Y}}^\dagger \begin{pmatrix} 1+r \\ (\mathbf{Y}_1^\dagger)^{-1}\vec{\psi}_1 \\ (\mathbf{Y}_2^\dagger)^{-1}\vec{\psi}_2 \\ \vdots \\ (\mathbf{Y}_l^\dagger)^{-1}\vec{\psi}_l \\ t_T \end{pmatrix} = \begin{pmatrix} -2i\sin q \\ \vec{0} \\ \vec{0} \\ \vdots \\ \vec{0} \\ 0 \end{pmatrix}. \tag{A.31}$$

Define $\mathbf{M}_l = \hat{\mathbf{X}}\mathbf{N}_l\hat{\mathbf{Y}}^\dagger$=

$$\begin{pmatrix} \xi & \vec{w}^\dagger\mathbf{Y}_1^\dagger & \vec{0}^\dagger & \vec{0}^\dagger & \cdots & \vec{0}^\dagger & \vec{0}^\dagger & 0 \\ \mathbf{X}_1\vec{w} & \mathbf{X}_1\mathbf{F}_1\mathbf{Y}_1^\dagger & \mathbf{X}_1\mathbf{B}_{12}\mathbf{Y}_2^\dagger & \mathbf{0} & \cdots & \mathbf{0} & \mathbf{0} & \vec{0} \\ \vec{0} & \mathbf{X}_2\mathbf{B}_{21}\mathbf{Y}_1^\dagger & \mathbf{X}_2\mathbf{F}_2\mathbf{Y}_2^\dagger & \mathbf{X}_2\mathbf{B}_{23}\mathbf{Y}_3^\dagger & \cdots & \mathbf{0} & \mathbf{0} & \vec{0} \\ \vec{0} & \mathbf{0} & \mathbf{X}_3\mathbf{B}_{32}\mathbf{Y}_2^\dagger & \mathbf{X}_3\mathbf{F}_3\mathbf{Y}_3^\dagger & \cdots & \mathbf{0} & \mathbf{0} & \vec{0} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ \vec{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{X}_{l-1}\mathbf{F}_{l-1}\mathbf{Y}_{l-1}^\dagger & \mathbf{X}_{l-1}\mathbf{B}_{l-1,l}\mathbf{Y}_l^\dagger & \vec{0} \\ \vec{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{X}_l\mathbf{B}_{l,l-1}\mathbf{Y}_{l-1} & \mathbf{X}_l\mathbf{F}_l\mathbf{Y}_l^\dagger & \mathbf{X}_l\vec{u} \\ 0 & \vec{0}^\dagger & \vec{0}^\dagger & \vec{0}^\dagger & \cdots & \vec{0}^\dagger & \vec{u}^\dagger\mathbf{Y}_l^\dagger & \xi \end{pmatrix}. \tag{A.32}$$

where $\mathbf{F}_l = \mathbf{A}_l - E\mathbf{I}$.

A successful mapping onto the 1D chain was defined by a set of equations

$$\mathbf{X_i}\mathbf{A_i}\mathbf{Y_i}^\dagger = \begin{pmatrix} \tilde{\epsilon}_i & \vec{0}^\dagger \\ \vec{0} & \tilde{\mathbf{A}}_i \end{pmatrix}. \tag{A.33}$$

$$\mathbf{X}_i\mathbf{B}_{ij}\mathbf{Y}_j^\dagger = \begin{pmatrix} -\tilde{t}_{ij} & \vec{0}^\dagger \\ \vec{0} & \tilde{B}_{ij} \end{pmatrix} . \tag{A.34}$$

$$E\mathbf{X}_i\mathbf{I}\mathbf{Y}_i^\dagger = \begin{pmatrix} E & \vec{0}^\dagger \\ \vec{0} & \tilde{C}_i(E) \end{pmatrix} . \tag{A.35}$$

$$\mathbf{X}_1\vec{w} = \begin{pmatrix} -\tilde{w} \\ \vec{0} \end{pmatrix} \quad \text{and} \quad \mathbf{Y}_1\vec{w} = \begin{pmatrix} -\vec{w} \\ \vec{0} \end{pmatrix} . \tag{A.36}$$

$$\mathbf{X}_l\vec{u} = \begin{pmatrix} -\tilde{u} \\ \vec{0} \end{pmatrix} \quad \text{and} \quad \mathbf{Y}_l\vec{u} = \begin{pmatrix} -\tilde{u} \\ \vec{0} \end{pmatrix} . \tag{A.37}$$

After the mapping, some hopping terms in the $\mathbf{M}_l$ become zero, which means that in the mapped structure, some atoms are disconnected from the blob and leads. Define the $\tilde{\mathbf{M}}_l$ as the matrix that includes all the connected atoms in the mapped structure.

$$\tilde{\mathbf{M}}_l = \begin{pmatrix} \xi & -\tilde{w} & 0 & 0 & \cdots & 0 & 0 & 0 \\ -\tilde{w} & \tilde{k}_1 & -\tilde{t}_{12} & 0 & \cdots & 0 & 0 & 0 \\ 0 & -\tilde{t}_{21} & \tilde{k}_2 & -\tilde{t}_{23} & \cdots & 0 & 0 & 0 \\ 0 & 0 & -\tilde{t}_{32} & \tilde{k}_3 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & \tilde{t}_{l,l-1} & -\tilde{k}_l & -\tilde{u} \\ 0 & 0 & 0 & 0 & \cdots & 0 & -\tilde{u} & \xi \end{pmatrix} . \tag{A.38}$$

where $\tilde{k}_i = \tilde{\epsilon}_i - E$.

To have quantum dragons in this nanodevice, one needs to set that

$$\tilde{w} = \tilde{u} = \tilde{t}_{i,i+1} = t_0 \tag{A.39}$$

and

$$\tilde{\epsilon}_i = \epsilon_0 \tag{A.40}$$

where t_0 is the hopping term between two lead atoms and ϵ_0 is the onsite energy of the lead atoms.

The idea underneath Eq. (38) and Eq. (39) is to set the mapped structure to be the same as lead so that the mapped structure can be seen as a continuous part of the lead. In this way the whole nanostructure will have total transmission. Since the mapped structure has the same solution about transmission as the original structure, therefore one can conclude that the original structure permits total electron transmission, namely a single-channel quantum dragon.