Time-Dependent Phonon-Assisted Tunneling through a Single-Molecular Device: Ricatti Matrix Approach

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Prelude

Today’s sophisticated modern microfabrication and self-assembly techniques → experiments aimed at probing the role of inelastic scattering in electron transport through very small single-molecular devices and semiconductor quantum dots.
Some simple systems:
eigenenergies:

\[ \varepsilon_c(s) = -2t_2 \cos k_c \]

\[ k_c = \frac{2\pi n}{s} \quad (n = 0, 1, 2, \ldots, s - 1) \]
eigenenergies:

\[ \varepsilon_c(s) = -2t_2 \cos k_c \]

\[ k_c = \frac{2\pi}{s} (n - f) \quad (n = 0, 1, 2, \ldots, s - 1) \]
The diagram shows the function $T(\varepsilon, \varepsilon')$ for different values of $f$. The function values range from 0 to 1, and the variable $\varepsilon$ is plotted on the x-axis, ranging from -2 to 2. The parameter $f$ varies from 0.0 to 1.0 in steps of 0.1.
WAVE FUNCTION VALUES AT THE JUNCTIONS

\[ \exp[ikx] + r \exp[-ikx] \quad a_n \exp[ikx] + b_n \exp[-ikx] \quad t \exp[ikx] \]

Point A is the origin of incident and middle circuits and point B is that for the outgoing circuit.
Results of experiments:

- Interactions between electrons and longitudinal optical phonons have substantial, rather than perturbational, effects on the transport properties of the mesoscopic device under question.
Single-molecular devices:

- Weak elastic parameters $\rightarrow$ low-energy vibrational modes.

- Strong coupling between these modes & electronic states of device $\rightarrow$ readily excited low-energy phonons, even at low temperatures while electron tunnels through device $\rightarrow$ phonon-assisted transport
Theoretical efforts:

- Many theoretical efforts to explore more the transport problem in the presence of electron-phonon interactions and/or other types of excitations.

- Some techniques: Green's function techniques, Fermi golden rule, pruning technique, kinetic-equation approach, and first-principles calculations.
Some important works of J. Bonca and coworkers (pruning technique):

Time-dependent case:

- Comparatively less investigated.

- Periodic time dependence is especially important → increased # of extra parameters (strength and period of excitation), in addition to already available parameters (strength of electron-phonon coupling and phonon frequency) → provides the researcher with a system which is more flexible in engineering it according to any desired particular needs.
An important work (pruning technique + Green’s function technique)

  time-averaged transmission displays additional peaks because of photon absorption/emission processes and photon-absorption-assisted phonon emission processes.
What we did:

A tight-binding model is studied to capture the essence of resonant transport of an electron through a single quantum-dot in the presence of both a time-periodic potential and phonon degrees of freedom.
Ricatti matrix method:

A non-perturbative pruning technique, combining the tight-binding scheme and the Floquet theory into a two-point recursive matrix equation.
System under study
- **system**: central site \((j=0)\), left \((j<0)\) and right \((j>0)\) leads.

- **central site**: Einstein phonons with frequency \(\Omega\) & time-periodic potential with period \(\tau=\frac{2\pi}{\omega}\).

- **ballistic one-electron picture**: no many-body effects like the Coulomb repulsion/blockade, spin-spin interaction, and phonon-mediated electron-electron interaction.
Hamiltonian of the system

\[ H(t) = \sum_j \left[ v_j(t)c_j^+c_j - \Delta_{j,j+1} c_j^+c_{j+1} - \Delta_{j,j-1} c_j^+c_{j-1} \right] + \Omega a^+a - \lambda c_0^+c_0(a^+ + a) \]
Applied potentials

\[
v_{j<0}(t) = v_L = \text{const.}, \quad v_{j>0}(t) = v_R = \text{const.}
\]

\[
v_{j=0}(t) = v_s + 2v_d \cos(\omega t)
\]

\[
H(t + \tau) = H(t) \quad \rightarrow \quad \text{time-periodic}
\]

\[
\tau = 2\pi / \omega
\]
Polaron eigenstates are used as basis [after Haule & Bonca, PRB 59, 13087 (1999)] → mapping a many-body problem exactly onto an effective one-body problem:

\[ |jm\rangle = \frac{1}{\sqrt{m!}} c_j^+ (a^+)^m |0\rangle \]

\[ m \geq 0 \]
Total wave function:

\[ \Psi(t) = \sum_{j,m} \psi_{j}^{(m)}(t) | jm \rangle \]
Time-dependent Schrödinger equation:

\[ i \frac{\partial}{\partial t} \Psi(t) = H(t) \Psi(t) \]
\[
i \frac{\partial}{\partial t} \psi_j^{(m)}(t) = [v_j(t) + m\Omega] \psi_j^{(m)}(t)
\]

\[
- \Delta_{j,j+1} \psi_{j+1}^{(m)}(t) - \Delta_{j,j-1} \psi_{j-1}^{(m)}(t)
\]

\[
- \delta_{j0} \lambda \left[ \sqrt{m+1} \psi_j^{(m+1)}(t) - \sqrt{m} \psi_j^{(m-1)}(t) \right]
\]
Floquet theory:

The **Floquet theorem** states that the solutions of 1D Schrödinger equation in a time periodic potential with period $T$ can be described as a linear combination of the **Floquet states**: 

$$
\varphi(x,t) = \sum_{\alpha} C_{\alpha} \varphi_{\alpha}(x,t), \quad \varphi_{\alpha}(x,t) = \exp(-i\varepsilon_{\alpha} t / \hbar) \phi_{\alpha}(x,t),
$$

$$
\phi_{\alpha}(x,t) = \phi_{\alpha}(x,t + T)
$$

where the function $\phi_{\alpha}$ is referred to as a **Floquet mode**. (This is so similar to Bloch states in solid state physics, where the periodic crystal environment is important.)
Floquet ansatz:

\[ \psi_j^{(m)}(t) = e^{-iEt} \phi_j^{(m)}(t) \]

\[ \psi_j^{(m)}(t) = e^{-iEt} \sum_{p=-\infty}^{\infty} e^{-ip\omega t} \phi_j^{(m,p)} \]
Solutions for leads:

\[ \phi_{j<0}^{(m,p)} = \delta_{mn} \delta_{pq} e^{i(j+1)k_L^{(n,q)}} + r^{(m,p)} e^{-i(j+1)k_L^{(m,p)}} \]

\[ \phi_{j>0}^{(m,p)} = t^{(m,p)} e^{-i(j-1)k_R^{(m,p)}} \]

\((n,q) : \text{initial channel}\)
Wave vectors:

\[ E = \nu_L + n \Omega - q \omega - 2\Delta \cos k_L^{(n,q)} \]

\[ = \nu_{L(R)} + m \Omega - p \omega - 2\Delta \cos k_{L(R)}^{(m,p)} \]

\[ \varepsilon = -2\Delta \cos k_L^{(n,q)}, \quad \varepsilon' = -2\Delta \cos k_R^{(m,p)} \]
Transform to matrix form:

Keeping site index $j$ fixed, every different combination $(m,p)$ leads to a different equation. We write all of them together in a matrix form:

$$
\tilde{E} \tilde{\Phi}_j = \tilde{V} \tilde{\Phi}_j - \tilde{\Delta}_{j,j+1} \tilde{\Phi}_{j+1} - \tilde{\Delta}_{j,j-1} \tilde{\Phi}_{j-1}
$$
Matrix dimensions:

\[ \tilde{X} : d \times d \]

\[ \tilde{X} : d \times 1 \]

\[ d = (m + 1)(2p + 1) \]
Matrix definitions

\[
[\tilde{E}]_{m,p;m',p'} = (E + p\omega - m\Omega)\delta_{mm'} \delta_{pp'}
\]

\[
[\tilde{\Delta}_{j\pm1}]_{m,p;m',p'} = \Delta_{j\pm1} \delta_{mm'} \delta_{pp'}
\]

\[
[V_j]_{m,p;m',p'} = (1 - \delta_{j0})v_{L(R)} \delta_{mm'} \delta_{pp'}
\]

\[
+ \delta_{j0} \left[ v_s \delta_{mm'} \delta_{pp'} + v_d \left( \delta_{mm'} \delta_{p-1,p'} + \delta_{mm'} \delta_{pp'-1} \right) - \lambda \left( \sqrt{m'} \delta_{m-1,m'} \delta_{pp'} + \sqrt{m} \delta_{m,m'-1} \delta_{pp'} \right) \right]
\]
We also write the solutions in matrix form:

\[
\phi_{j<0}^{(m,p)} = \delta_{mn} \delta_{pq} e^{i(j+1)k_L^{(n,q)}} + r^{(m,p)} e^{-i(j+1)k_L^{(m,p)}}
\]

\[
\phi_{j>0}^{(m,p)} = t^{(m,p)} e^{i(j-1)k_R^{(m,p)}}
\]

\[
\tilde{\Phi}_{j<0} = \tilde{a}_j + \tilde{b}_j \tilde{r}
\]

\[
\tilde{\Phi}_{j>0} = \tilde{c}_j \tilde{t}
\]
Matrix definitions:

\[
\begin{align*}
\left[ \tilde{a}_j \right]_{m,p;1} &= e^{i(j+1)k_L^{(n,q)}} \delta_{mn} \delta_{pq} \\
\left[ \vec{b}_j \right]_{m,p,m',p'} &= e^{-i(j+1)k_L^{(m,p)}} \delta_{mm'} \delta_{pp'} \\
\left[ \vec{c}_j \right]_{m,p,m',p'} &= e^{i(j-1)k_R^{(m,p)}} \delta_{mm'} \delta_{pp'} \\
\left[ \tilde{r} \right]_{m,p;1} &= r^{(m,p)} \\
\left[ \tilde{t} \right]_{m,p;1} &= t^{(m,p)}
\end{align*}
\]
Two important works which use Ricatti method:

- J. Heinrichs, PRB 65, 075112 (2002).
Ricatti matrix definition:

\[ \tilde{\Phi}_{j+1} = \tilde{Y}_j \tilde{\Phi}_j \]
Ricatti matrix equation:

\[
\tilde{E} \tilde{\Phi}_{j} = \tilde{V} \tilde{\Phi}_{j} - \tilde{\Delta}_{j,j+1} \tilde{\Phi}_{j+1} - \tilde{\Delta}_{j,j-1} \tilde{\Phi}_{j-1} \\
\tilde{\Phi}_{j+1} = \tilde{Y}_{j} \tilde{\Phi}_{j} \\
\Downarrow \\
\tilde{Y}_{j-1} = \left( \tilde{V}_{j} - \tilde{E} - \tilde{\Delta}_{j,j+1} \tilde{Y}_{j} \right)^{-1} \tilde{\Delta}_{j,j-1}
\]
Transmission and reflection amplitude matrices:

\[ \tilde{\Phi}_{j<0} = \tilde{a}_j + \tilde{b}_j \tilde{r}, \quad \tilde{\Phi}_{j>0} = \tilde{c}_j \tilde{t} \]

\[ \tilde{\Phi}_{j+1} = Y_j \tilde{\Phi}_j \]

\[ \tilde{t} = Y_0 Y_{-1} (\tilde{a}_{-1} + \tilde{r}) \]

\[ \tilde{r} = \left(Y_{-2}^{-1} - \tilde{b}_{-2}\right)^{-1} \left(\tilde{a}_{-2} - \tilde{b}_{-2} \tilde{a}_{-1}\right) - \tilde{a}_{-1} \]
Transmission amplitude matrix:

\[ \tilde{t} = \tilde{Y}_0 \tilde{Y}_{-1} (\tilde{a}_{-1} + \tilde{r}) \]

\[ \tilde{r} = \left( \tilde{Y}_{-2}^{-1} - \tilde{b}_{-2} \right)^{-1} \left( \tilde{a}_{-2} - \tilde{b}_{-2} \tilde{a}_{-1} \right) - \tilde{a}_{-1} \]

\[ \tilde{t} = \tilde{Y}_0 \tilde{Y}_{-1} \left( \tilde{Y}_{-2}^{-1} - \tilde{b}_{-2} \right)^{-1} \left( \tilde{a}_{-2} - \tilde{b}_{-2} \tilde{a}_{-1} \right) \]
Initial datum:

\[ \tilde{\Phi}_2 = \tilde{Y}_1 \tilde{\Phi}_1 \rightarrow \tilde{c}_2 \tilde{t} = \tilde{Y}_1 \tilde{t} \]

\[ \Downarrow \]

\[ \tilde{Y}_1 = \tilde{c}_2 \]
Scenario:

\[ \vec{Y}_1 = \vec{c}_2 \rightarrow \text{initial data} \]

\[ \vec{Y}_{j-1} = \left( \vec{V}_j - \vec{E} - \Delta_{j,j+1} \vec{Y}_j \right)^{-1} \Delta_{j,j-1} \rightarrow \vec{Y}_0 \rightarrow \vec{Y}_{-1} \rightarrow \vec{Y}_{-2} \]

\[ \tilde{t} = \vec{Y}_0 \vec{Y}_{-1} \left( \vec{Y}_{-2}^{-1} - \vec{b}_{-2} \right)^{-1} \left( \vec{a}_{-2} - \vec{b}_{-2} \vec{a}_{-1} \right) \]
Transmission matrix:

\[
\left[ \tilde{T}(\varepsilon, \varepsilon') \right]_{(n,q)\rightarrow(m,p)} = \left| \tilde{t} \right|^{2} \frac{\sin k_R^{(m,p)}}{\sin k_L^{(n,q)}}
\]
Temperature effect:

\[ P(n) = \left( 1 - e^{-\beta \Omega} \right) e^{-n \beta \Omega} \]
Total transmission:

\[
T_{\text{tot}}(\varepsilon) = \sum_{n,m} \sum_{q,p} P(n) \left[ \vec{T}(\varepsilon, \varepsilon') \right]_{(n,q) \rightarrow (m,p)}
\]
Some representative results:

\[ v_L = v_R = 0 \]

initial channel: \((n, q = 0)\)
final channel: \((m, p)\)

\[ N_\omega = N_\Omega = 10 \rightarrow \text{maximum # of channels} \]
Eigenvalues, only time-dependent case:

\[ \varepsilon \approx \kappa \omega \]

\[ \kappa = 0, \pm 1, \pm 2, \ldots \]
Eigenvalues, only phonon case:

\[ \varepsilon \approx -\lambda^2 / \Omega + \ell \Omega \]

\[ \ell = 0, \pm 1, \pm 2, \ldots \]
\[ \lambda = 0.2 \]
\[ \Omega = 0.4 \]
\[ \Delta = 1.0 \]
\[ \Delta_0 = 0.2 \]

The graph shows the total temperature \( T_{\text{total}}(\epsilon) \) as a function of \( \epsilon \), with different lines indicating various values of \( T \):

- \( T = 0.00 \)
- \( T = 0.25 \)
- \( T = 0.50 \)
- \( T = 1.00 \)
Eigenvalues, combined effect:

\[ \varepsilon \approx -\lambda^2 / \Omega + \ell \Omega + k \Omega \]
$\lambda = 0.2$

$\Omega = 0.4$

$v_s = 0.0$

$v_d = 0.1$

$\omega = 0.25$

$\Delta = 1.0$

$\Delta_0 = 0.2$
Conclusions:

- We offer the use of the Ricatti matrix method, a numerically exact method, to study the resonant tunneling of an electron through a single quantum-dot in the presence of both an oscillating potential and electron-phonon interaction.
Conclusions:

The presented method merges the tight-binding and the Floquet theory into a two-point recursive matrix equation; it is essentially a powerful non-perturbative pruning technique.
Conclusions:

- In this work we placed the particular importance on its derivation for the simplest system possible; it can be easily generalized to study more complicated similar systems.
Conclusions:

- As an immediate example, by making use of the decimation technique [H.M. Pastawski & E. Medina, Rev. Mex. Fis. 47, 1 (2001)], this method can be successfully utilized in investigating Aharonov-Bohm type quasi two-dimensional electron pump systems with or without electron-phonon interactions, or with any type of similar inelastic interactions.
Conclusions:

- Its simple-to-comprehend and easy-to-implement properties, and its capability of producing essentially exact numerical results render Ricatti matrix method promising for studying more complicated similar systems.
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Time-dependent phonon-assisted tunneling through a single-molecular device: Ricatti matrix approach

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Abstract. – We study a tight-binding model to capture the essence of resonant transport of an electron through a single quantum-dot in the presence of both a time-periodic potential and phonon degrees of freedom. In order to solve the time-dependent Schrödinger equation we use a non-perturbative pruning technique, called Ricatti matrix method, which combines the tight-binding scheme and the Floquet theory into a two-point recursive matrix equation. Its simple-to-comprehend and easy-to-implement properties, and its capability of producing essentially exact numerical results render Ricatti matrix method promising for studying more complicated similar systems.

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Introduction. – With the aid of modern micro-fabrication and self-assembly techniques, it has become a commonplace to see experiments aimed at probing the role of mesoscopic scattering in electron transport through very small single-molecular devices and semiconductor quantum dots [1,2]. It follows from these studies that interactions between electrons and longitudinal optical phonons has substantial, rather than perturbational, effects on the transport properties of the mesoscopic device under question. In particular, owing to their weak elastic parameters, single-molecular devices have low-energy vibrational modes. The strong coupling between these modes and the electronic states of the device causes the low-energy phonons to be readily excited even at low temperatures while the electron tunnels through the device [1-3]. This phenomenon has been known as the phonon-assisted transport and has always given a constant impetus to researchers; during the last two decades the literature has witnessed a good number of theoretical efforts to explore more the transport problem in the presence of electron-phonon interactions and/or other types of excitations. These works were based on the nonequilibrium Green’s function technique [4-9], the Fermi golden rule [10], the pruning technique [11-13], the kinetic-equation approach [14-16] and first-principles calculations [17].

Most of the mentioned theoretical works concentrated on the stationary electron-phonon problem; the time-dependent cases have been comparatively less investigated. The inclusion of time-dependent excitations, especially time-periodic ones, into the phonon-assisted tunneling bears particular importance. Such a periodic time dependence gives rise to a number of extra parameters, like the strength and period of excitation, in addition to the already available parameters, like the strength of electron-phonon coupling and phonon frequency. This, in turn, will certainly provide the researcher with a system which is now more flexible in engineering it according to any desired particular needs. In a recent significant work, Dong et al. [3] have investigated the problem of time-dependent phonons-assisted tunneling through a single-molecular quantum dot by making use of nonequilibrium Green’s function technique which was based on a pruning technique [11]; it has been reported that the time-averaged transmission has displayed additional peaks because of photon absorption/emission processes, and so has the nonlinear differential permanence due to photon-absorption-assisted phonon emission processes. It thus seems that studying the time-dependent phonon-assisted tunneling is especially beneficial. The principal objective of the present work is to further investigate the resonant electron transport problem in the presence of both a time-periodic potential and electron-phonon interaction using a different computational approach, called Ricatti matrix method, which simplifies greatly solving the time-dependent Schrödinger equation.

Method. – The system we study in the present work is composed of a central site (j = 0) and the left (j < 0)
An application of this method for an Aharonov-Bohm ring appeared in "J. Phys.: Condens. Matter 19, 226211 (2007)."
Phonon–photon-assisted tunnelling through an Aharonov–Bohm ring

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Abstract
We model a four-site tight-binding Aharonov–Bohm (AB) ring whose sites house dispersionless Einstein phonons. The resonant tunnelling of an electron through the AB ring in the presence of a time-periodic magnetic flux which threads the ring is investigated. The Floquet scattering approach is followed within the electron–phonon Fock space. The Ricatti matrix method, a nonperturbative pruning technique, is utilized to extract the transmission properties of the system from the time-dependent Schrödinger equation. We observe additional satellite peaks in the total transmission graphs representing the photon-assisted tunnelling, as well as side resonances due to the phonon-assisted tunnelling. There happen to exist unusually stiff main transmission peaks that are not disturbed by the strong time-periodic magnetic flux, a finding attributed to the geometric characteristics of the AB ring.

1. Introduction

Recent advances in nanotechnologies have directed scientific attention to the study of the electron transport through very small mesoscopic structures, such as a quantum dot, quantum wire, and Aharonov–Bohm (AB) ring. In these systems, whose geometrical dimensions are much smaller than the elastic mean free path, electrons are transported ballistically and many interesting quantum coherent phenomena are observed [1]. As a standard method for probing the coherence, many experimentalists have made use of AB interferometers, and recently there has been a growing interest in hybrid systems composed of an AB interferometer and quantum dots [2–5]. One of the motivations for our work comes from the fact that it is possible at the present to embed quantum dots in the arms of AB rings, and perform quantum interference experiments in such systems [4, 5]. Electron waves on the dots scatter, leading a phase shift which is additional to the usual interference of the waves from the upper and lower part of the ring.

With the rapid progress of miniaturization, molecular electronics has become a subject of special interest in many branches of physics, chemistry, and biology [6]. A recent molecular
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Once upon a time my dear colleagues in Seoul Nat’l University

D. Shin, J. Hong, W. Woo
Once upon a time my dear colleagues in Seoul Nat’l University
Dedicated to

Prof. Dr. Şakir Erkoç,

whom I venerate as my master, nor did I ever regret it from the very first day I got to know him ...