Simulation of Quantum Wires with Resonant Transmission Lines

C. D. Papageorgiou, T. E. Raptis and A. C. Boucouvalas

Abstract—We use the previously introduced Resonant Transmission Line (RTL) method for numerically tackling the problem of a 1D quantum wire with arbitrary curvature allowing fast, efficient computation of both eigenvalues and eigenfunctions. Analysis reveals a strict dependency of the energy eigenvalues to the curvature magnitude with significant lowering and even vanishing of the first harmonic beyond a threshold value which severely affects excitability of each eigenfunction .

***Keywords*—**Schrödinger equation, transmission line

I. Introduction

IN a recent series of publications Stockhofe and Schmelcher [1] as well as Zambetaki *et al.*, [2] propose a treatment of the Schrodinger equation in a curvilinear coordinate system for one dimensional quantum waveguides.

We examine this recently introduced case of the Schrodinger equation on a curved one dimensional path, in the light of the proposed Resonant Transmission Line (RTL) simulation and the related numerical method. By a segmentation process we show how to extend this in the case of any curved wire of arbitrary curvature.

The calculation of eigenvalues is simplified using the resonance condition of the equivalent RTL and for each eigenvalue the eigenfuctions can be calculated also numerically. We show that for special shaped quantum wires the basic "Energy" of excitation can be reduced significantly.

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II. Description of the RTL Method

A generic equivalence of the Schrodinger problem or the general Sturm-Liouville problem in one dimension has been established in [3], [4] and [5], which is valid not only for ODE problems but also for PDEs in separable coordinate systems. To this aim, we consider the representation of a non homogeneous lossless transmission line defined along its geometric length s, with $V(s)$ and $I(s)$ its voltage and current values and X(s), Y(s) its "reactance" and "admittance" per length unit respectively. The general PDE representation of such a line is given as

$$\begin{cases} \partial_l V(s) = -jX(s)I(s) \\ \partial_l I(s) = -jY(s)V(s) \end{cases} \tag{1}$$

It is very easy to show that the set (1) is equivalent to the generic Sturm-Liouville equation

$$\partial_l \left(\frac{1}{Y(s)} \partial_l I(s) \right) = -j\partial_l(s) = -X(s)I(s) \tag{2}$$

This the exact same form of the corresponding Schrödinger operator under the identification of the wavefunction $y(s)$ with the current $I(s)$ and the voltage $V(s)$ with the expression $j\dfrac{1}{Y(s)}\partial_l y(s)$. Considering an infinitesimal length transmission line *ds* where both admittance and reactance can be taken as constant, the description becomes identical with that of the so called T-quadrupole circuit shown in fig 1.

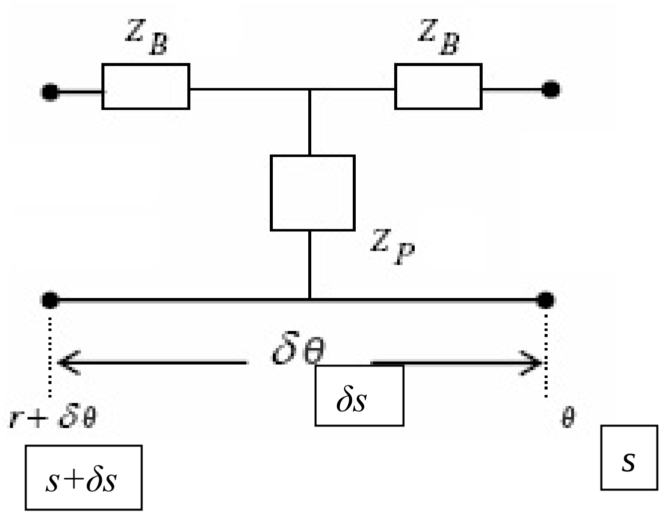

Fig. 1 Schematic of a 4-port T-circuit.

The respective impedances are then given as

$$\begin{cases} Z_B = Z\tanh(\gamma ds/2) \\ Z_P = Z/\sinh(\gamma ds) \end{cases} \tag{3}$$

In (3) we identify the local transmission factor as $\gamma(s) = j\sqrt{X(s)Y(s)}$ and the input impedance as $Z(s) = -j\gamma(s)/Y(s)$. For $\gamma(s)ds << 1$ we can always approximate this with a proper choice of the step ds as

$$\begin{cases} Z_B(s) = Z(s)\gamma(s)ds/2 = -j\gamma(s)^2 ds/2Y(s) \\ Z_P(s) = Z(s)/(\gamma(s)ds) = 1/(jY(s)ds) \end{cases} \tag{4}$$

A succession of such T-quardupoles can be used to approximate a transmission line with continuously varying parameters of reactance and admittance. In any real non homogeneous transmission line, both γ^2 as well as $Y(s)$ are functions of the excitation frequency ω associated with the energy parameter E. The frequency values, for which the whole line becomes tuned so as to achieve maximal power transmission, are the resonant values which stand for the line eigenvalues and the corresponding current values along the line are the line's eigenfunctions.

From the well known properties of transmission lines, for any such resonant line, the total reactances calculated from the left and right terminals towards any intermediate point must equal each other with opposite signs. Hence, the resonant values of frequencies or energies can be found from the roots of the total function with $L_{1,2}$ the total lengths towards any central point as

$$X_L(L_1) + X_R(L_2) = 0 \tag{5}$$

Given the terminal impedances, the left and right totals can be calculated for any E value.

Having found the eigenvalues from the roots of (5), it is equally possible to extract the exact shape of the eigenfunctions from the current values as follows. From the general theory of the telegrapher's equation we know that a solution via a transfer matrix can always be written in the form of a dynamical system $\mathbf{x}_n = \hat{T}_n \mathbf{x}_{n-1}$, where $\mathbf{x}_n = [V_n, I_n]$, the voltage-current vector and T_n an array of the form

$$\hat{T}_n = \begin{pmatrix} \cosh(\gamma(s)ds) & Z)(s)\sinh(\gamma(s)ds) \\ \sinh(\gamma(s)ds)/Z(s) & \cosh(\gamma(s)ds) \end{pmatrix}, \tag{6}$$
$$Z(s) = j\gamma(s)$$

In (6) we used $ds = x_n - x_{n-1}$.

III. Thin Curved Wires as Quantum Potential Wells

Without any external electric field acting on a quantum wire, free electrons will be affected by the wire's curvature and some deviation from the original smooth envelope of their eigenfunctions should be expected.

To analyze the situation we assume a parametric representation of the curve on which the wire lies given by three scalar functions of an abstract parameter s as $x(t)$, $y(t)$ and $z(t)$ and take a split into N sections by an arbitrary choice of t_1, …, t_N such that $\sqrt{\Delta x^2 + \Delta y^2 + \Delta z^2} < l_0$ with l_0 a sufficiently small length with $\Delta x_i = x_i(t_n) - x_i(t_{n-1})$ etc for Δy, Δz. Any individual section will then have its own radius of curvature R given by the relation (7)

$$(1/R)^2 = \frac{(\dot{y}\ddot{z} - \dot{z}\ddot{y})^2 + (\dot{z}\ddot{x} - \dot{x}\ddot{z})^2 + (\dot{x}\ddot{y} - \dot{y}\ddot{x})^2}{(\dot{x}^2 + \dot{y}^2 + \dot{z}^2)^3} \tag{7}$$

In (7), simple and double dots stand for the 1st ans 2nd derivatives with respect to the parameter t and their evaluation is taking place in the middle point of each section $(t_n + t_{n-1})/2$.

We can easily prove that the parameter t can always be replaced by the length s along the curved thin wire given by

$$s = \int_0^t \sqrt{x'^2 + y'^2 + z'^2} \cdot dt$$

This means that for any set of consecutive parameter values t_n the respective values of s_n and σ_n can be numerically calculated.

Thus at the present paper the curvature σ can be considered as function of the length parameter s.

The Schrödinger equation for a curved one dimensional (thin) wire developed along its parametric length s with $0 \le s \le L$ is given by

$$\partial^2 y(s)/\partial^2 s = -\left(\frac{\sigma^2(s)}{4}+\varepsilon\right)y(s),$$
$$\left(\frac{\sigma^2(s)}{4}+\varepsilon\right) = \left(\frac{1}{4R^2(s)}+\varepsilon\right)m/2\hbar^2 \quad (8)$$

In (8), the standard curvature is given by the local radius R via $\sigma(s) = 1/R(s)$. This, homogeneous, linear 2nd order ODE can be solved with the aid of the Resonant Transmission Line (RTL) technique previously introduced by Papageorgiou et.al in [3] and used already in a variety of other 2nd order ODEs and PDEs.

Following the analysis there, equation (1) reduces to the case of a transmission line with $\mathrm{Y}(s) = 1, \mathrm{X}(s) = \varepsilon + \sigma^2(s)/4$ which give the local propagation constant at each point as

$$\gamma^2(s) = -\left(\varepsilon + \sigma^2(s)/4\right) \quad (9)$$

We take every small part of the curved wire of length δs as equivalent to a T-quadrupole of impedances Z_B and Z_P with reference to figure 1, being given as

$$\begin{cases} Z_B(s) = -j\gamma(s)^2\delta s/2 \\ Z_P(s) = -j/\delta s \end{cases} \quad (10)$$

We also take the terminal impedances of the equivalent line at the boundaries s =0 and L to be infinite so as to make $y(s)$ zero at these points.

We now consider a varying curvature which introduces an equivalent effective potential of geometric origin and we compute the resulting eigenvalues and eigenfunctions. To this purpose, we divide the wire in small parts of length δs along which we may take the curvature to be practically constant.

Each such element is then equivalent to the T-quadrupole parametrized as in (2) and (3). The whole wire is then equivalent to a lossless non homogeneous transmission line made by the succession of T-quadrupoles terminated at infinite impedances. We now have the freedom to choose any arbitrary intermediate point and calculate the respective “left” and “right” impedances as functions of the energy ε. Eigenvalues will then correspond to the roots of the function $Z_L(\varepsilon) + Z_R(\varepsilon)$

The respective eigenfunctions are then directly obtained for each and any eigenvalue from the values of the respective currents of the T-quadrupoles through the application of a Transfer Matrix on a set of initial conditions as explained in App. A. in the form

$$\begin{bmatrix} U_{n+1} \\ I_{n+1} \end{bmatrix} = \begin{pmatrix} \cosh(\delta s_n\gamma_n) & Z_n\sinh(\delta s_n\gamma_n) \\ Z_n^{-1}\sinh(\delta s_n\gamma_n) & \cosh(\delta s_n\gamma_n) \end{pmatrix} \begin{bmatrix} U_n \\ I_n \end{bmatrix}$$
$$Z_n = -j\gamma_n$$
(11)

Initial values are taken as V_0 =1 and I_0 = 0. For infinitesimal displacements, (4) can always be approximated as

$$\begin{bmatrix} U_{n+1} \\ I_{n+1} \end{bmatrix} = \begin{pmatrix} 1 & -j\delta s_n\gamma_n^2 \\ j\delta s_n & 1 \end{pmatrix} \begin{bmatrix} U_n \\ I_n \end{bmatrix}, \quad Z_n = -j\gamma_n$$
(12)

The trajectory obtained this way contains the representation of the eigenfunction from the current values *[I_1, I_2,…I_n]* at the chosen points of the curved wire.

From quantum mechanical properties it is known that the square of $y(s_n) = I_n$, represents the expected probability of the free electron to be placed at the point s_n. Thus for a large number of free electrons of the curved wire the squared values of the set *[I_1, I_2,…I_n]* are giving the electric charge at the set of points *[s_1, s_2,…s_n]*.

We then naturally anticipate that under an external excitation there will be a tendency of free electrons to be present at these points proportionally to their squared “currents”. We performed a numerical exploration of the effects of curvature in the one dimensional wire model.

Since the first harmonic with the lower energy eigenvalue appears to be the most important for any energy transfer mechanism, as well as for the maximal concentration of the free electron density, we concentrate on this case.

For the first harmonic we expect to have two zeros at the terminal points (0, L) and a single maximum in an intermediate point. We chose to examine a case of a curved planar symmetric wire of length L = 1 subdivided in three areas as

$$\sigma(s) = \begin{cases} 0, & 0 \le s < L_1 \\ \dfrac{\varphi}{L-2L_1}, & L_1 \le s \le L - L_1 \\ 0, & L_1 < s \le L \end{cases} \quad (13)$$

The middle part corresponds to an arc with radius $R = (L - 2L_1)/\varphi$ while φ in stands for the arc angle. Results of our simulations are shown in figure 2 where the eigenvalue of the first harmonic is plotted as a function of the arc φ for the characteristic ratio $n_1 = 0.28$. Also in the figures 3,4,5 we show the first three eigenfunctions of curved quantum wires as described before with characteristics {n1=0.4 & φ =110^0}, {n1=0.25 & φ =180^0} ,{n1=0.1 & φ =270^0} are plotted. The relevant MATAB codes are shown in Appendix I

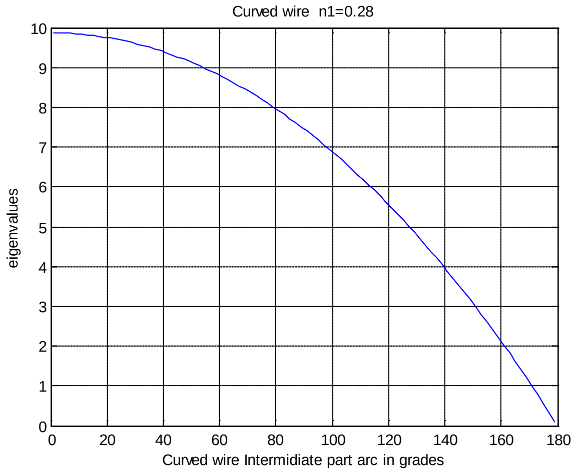

FIG. 2 CURVED WIRE SEGMENT FOR N1=0.28 IN GRADES.

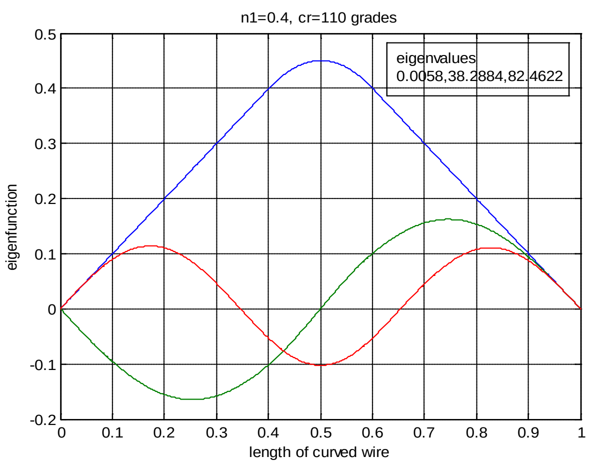

Fig. 3

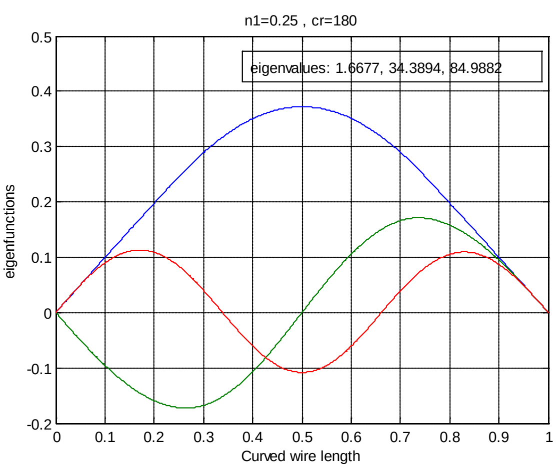

Fig. 4

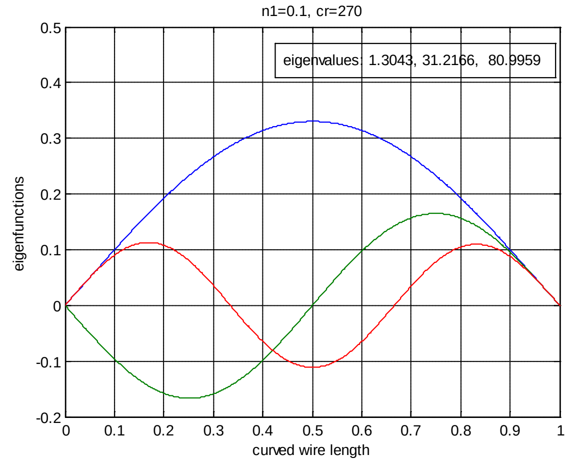

Fig. 5

IV. DISCUSSION AND CONCLUSIONS

By the previous analysis it becomes evident that the curvature effect results in a kind of amplification of the free electron concentration. The resulting lowering of the energy eigenvalue is also suggestive of the fact that lower external energy source can now more easily excite this particular fundamental mode. The authors intend to use and extend this analysis into the difficult subject of understanding the current distribution in excited curved antenna systems which remains largely unsolved. In a recent paper [6] we also proposed that this curvature effect of modified Li-Ion Batteries of a number of SAMSUNG Galaxy S7 mobiles, could be the main reason of their abrupt, catastrophic explosions.

APPENDIX

```
function fz=wirezero1
% calculates the eigenvalues of the curved
symmetric wire of length=1
% Of two rectilinear parts of length n1
% And a central curved part of length 1-
2n1 and of angle cr (in grades)
% using the function wire2

global n1 cr fy

N=1000;
N1=n1*N;
N2=N-2*N1;
fz=0;
for n=1:2001;x(n)=(n-1)/20;
    y(n)=wire2(x(n));end
L=0;
for n=1:2000; yy(n)=y(n)*y(n+1);
 if yy(n)<0 && y(n)>0;L=L+1;
       fz(L)= fzero(@wire2,[x(n),x(n+1)]);
    end
end
fy=fz;



function y=wire2(e)
```

```
% root finder for a curved wire of length
1, with two symetric equal
% rectilinear parts of n1<0.5 length, and
an intermediate curved part of N2/N
% length, with a radious  R extending in
an angle cr=(angle in degrees)

global n1 cr

N=1000;
N1=n1*N;
N2=(N-2*N1);
dz=1/N;
R=(N2/N)/(cr*(pi/180));
zz=10^8;
for n=1:N1+N2;
    w1=0;
    x=N*dz-(n-1)*dz+dz/2;
   if n>N1;
       w1=1/4/R^2;
    end
    cc=-e-w1;
    zb=j*cc*dz/2;
    zp=j/dz;
    zz=(zz+zb)*zp/(zz+zb+zp)+zb;

end
z1=zz;
zz=10^8;
for n=1:N1;

    x=N*dz-(n-1)*dz+dz/2;
    cc=-e;
    zb=j*cc*dz/2;
    zp=j/dz;
    zz=(zz+zb)*zp/(zz+zb+zp)+zb;
end
y=imag(zz+z1);


function wire33
%eigenfunction for a given eigenvalue on a
wire described by wire1 function

global fy xx yy rr ww
for nn=1:3
    e=fy(nn);
N=1000;
dz=1/N;

zz=[1;0];
f(1)=zz(2);
xx(1)=1;
for n=1:N;
    x=N*dz-(n+1/2)*dz;
    xx(n+1)=x+dz/2;
    cc=-wire1(x)-e;
    A=[1 -j*cc*dz;j*dz 1];
    zz=A*zz;
    f(n+1)=zz(2);

end
if nn==1;yy=imag(f);end;
if nn==2;rr=imag(f);end
if nn==3;ww=imag(f);end
end
yy(1)=0;rr(1)=0;ww(1)=0;
plot(xx,yy,xx,rr,xx,ww);grid on


function y=wire1(x)
% The Geometric potential of a curved wire
length 1 of two recilinear parts
% of length n1<0.5 and one curved
intermediate part of length N2/N of
constant
% curvature 1/R ;cr=angle of the curved
part in degrees (180 degrees=pi)
global n1 cr
N=1000;
N1=n1*N;
N2=(N-2*N1);
dz=1/N;
R=(N2/N)/(pi*cr/180);
n=x/dz;
    y=0;
     if n>N1 && n<N1+N2;
      y=1/4/R^2;
    end
```

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