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Quantum motion over a finite one-dimensional domain: With and without dissipation

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Abstract. Quantum motion of a single particle over a finite one-dimensional spatial domain is considered for the generalized four parameter infinity of boundary conditions (GBC) of Carreau *et al* [1]. The boundary conditions permit complex eigenfunctions with nonzero current for discrete states. Explicit expressions are obtained for the eigenvalues and eigenfunctions. It is shown that these states go over to plane waves in the limit of the spatial domain becoming very large. Dissipation is introduced through Schrödinger–Langevin (SL) equation. The space and time parts of the SL equation are separated and the time part is solved exactly. The space part is converted to nonlinear ordinary differential equation. This is solved perturbatively consistent with the GBC. Various special cases are considered for illustrative purposes.

Keywords. Generalized boundary conditions; free particle; finite domain; dissipation; Schrödinger–Langevin equation.

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1. Introduction

Recently Carreau *et al* [1] has shown that a four parameter infinity of generalized boundary conditions (GBC) exist for the case of a free motion in one dimension over a finite spatial domain. These boundary conditions admit complex wave functions with nonzero current as eigenstates. Such states can find a natural application in many physical problems such as motion of an electron confined in a quantum well or quantum tunneling across a Josephson junction. In most such practical cases dissipation plays an important role. There are two types of approaches to study quantum dissipative systems. In one approach the central system of interest is coupled to extra degrees of freedom and although the total system remains conservative, elimination of the extra degrees of freedom in an appropriate approximation makes the central system dissipative [2, 3]. In the other approach phenomenological quantum equations displaying dissipative behaviour are used. In this category comes the well known Schrödinger–Langevin (SL) equation [4], Gisin equation [5] and the use of complex potential [6]. We report the free particle eigenspectrum explicitly using the GBC and show how the discrete states go over to the plane waves as the spatial domain size increases indefinitely. We introduce dissipation through the SL equation and separate its time and space parts. The time part is solved exactly and the space part is reduced to a nonlinear ordinary differential equation. A special solution of this equation is obtained and the problems of applying GBC are pointed out. A perturbative scheme for solving the space part consistent with the GBC is developed.

2. Particle in a 1-dimensional box with GBC

Consider a nonrelativistic particle of mass m confined to a spatial domain $0 < x < L$. The commonly used boundary conditions on the wave function are

$$\psi(0) = 0 = \psi(L). \tag{2.1}$$

A more general class of boundary conditions are [1, 7]

$$\begin{bmatrix} -\psi'(L) \\ \psi'(0) \end{bmatrix} = M \begin{bmatrix} \psi(L) \\ \psi(0) \end{bmatrix}, \tag{2.2}$$

where the prime denotes differentiation with respect to x and M is a 2×2 Hermitean matrix

$$M = \begin{bmatrix} a & \alpha + i\delta \\ \alpha - i\delta & b \end{bmatrix}. \tag{2.3}$$

a, b, α and δ are the four real parameters. Using (2.2) it readily follows that the energy eigenvalues are given by

$$E_k = \frac{\hbar^2 k^2}{2m}, \tag{2.4}$$

with k satisfying the dispersion relation

$$2k\alpha + (a+b)k\cos(kL) + [ab - \alpha^2 - \delta^2 - k^2]\sin(kL) = 0. \tag{2.5}$$

The corresponding wave function is given by

$$\psi_k(x) = A[\sin(kx) + C\cos(kx)] \tag{2.6}$$

with

$$C = \frac{[k - (\alpha - i\delta)\sin(kL)]}{[b + (\alpha - i\delta)\cos(kL)]} \tag{2.7}$$

and the constant A is obtained from normalization.
The state (2.6) has a nonzero current

$$j_k = |A|^2 \left(\frac{\hbar k}{m}\right) \delta \frac{[k\cos(kL) + b\sin(kL)]}{\{[b + \alpha\cos(kL)]^2 + \delta^2\cos^2(kL)\}}. \tag{2.8}$$

The usual boundary conditions (2.1) are special cases of (2.2) when

$$a \to \infty, \quad b \to \infty, \quad \alpha \to 0, \quad \delta \to 0. \tag{2.9}$$

It is interesting to consider the large L limit. For usual boundary conditions the states remain discrete and the current zero. Physically, this can be attributed to the fact that any eigenstate is an equal weight linear combination of plane waves moving from left to right and vice versa. Unless an imbalance is introduced in these waves, nonzero current is not possible. GBC introduces such an imbalance and it is readily shown that

$$\lim_{L\to\infty} C = \frac{1}{L}\int_{L}^{2L}\frac{[k-(\alpha-i\delta)\sin(kx)]\mathrm{d}x}{[b+(\alpha-i\delta)\cos(kx)]}\to \pm i \tag{2.10}$$

so that the wave function (2.6) goes over to $\exp(\pm ikx)$.

3. Schrödinger–Langevin equation: *t*-dependence

We now consider dissipative motion over the domain $0 < x < L, 0 < t < \infty$ for the free particle using the SL equation

$$i\hbar\partial\psi/\partial t = -\frac{\hbar^2}{2m}\partial^2\psi/\partial x^2 + \frac{\lambda\hbar}{2i} ln[\psi/\psi^*]\psi, \tag{3.1}$$

where λ is the dissipation coefficient. The space and time parts of the wave function can be separated by putting

$$\psi(x,t) = \phi(x)\chi(t). \tag{3.2}$$

$\chi(t)$ and $\phi(x)$ then satisfy

$$i\hbar\mathrm{d}\chi/\mathrm{d}t = \frac{\lambda\hbar}{2i}\ln[\chi/\chi^*]\chi + W\chi \tag{3.3}$$

and

$$-\frac{\hbar^2}{2m}\mathrm{d}^2\phi/\mathrm{d}x^2 + \frac{\lambda\hbar}{2i}\ln[\phi/\phi^*]\phi = W\phi. \tag{3.4}$$

W is the separation constant and in general it can be complex. We first consider the time part (3.3) which can be readily integrated to give the solution

$$\chi(t) = \exp(W_{\mathrm{I}}t/\hbar)\cdot\exp[-iG_{\mathrm{R}}(t)/\hbar], \tag{3.5}$$

were W_{I} is the imaginary part of W and the real function G_{R} satisfies the differential equation

$$\mathrm{d}G_{\mathrm{R}}/\mathrm{d}t + \lambda G_{\mathrm{R}} = W_{\mathrm{R}}, \tag{3.6}$$

W_{R} being the real part of the separation constant W.

Thus when $W_{\mathrm{I}} > 0$ (2.5) blows up with time t and when $W_{\mathrm{I}} < 0$ it decays to zero. The first case is evidently unphysical and the second is a well known difficulty with quantum dissipative systems [3, 6]. A special solution exists for the spatial part when W_{I} has a particular negative value as discussed in the next section.

The most general solution of (3.6) is given by

$$G_{\mathrm{R}}(t) = \frac{W_{\mathrm{R}}}{\lambda}[1-\exp(-\lambda t)] + G_0\exp(-\lambda t), \tag{3.7}$$

where G_0 is an arbitrary constant. From (3.5), W_{I} can be thought of as the imaginary part of particle energy and $\mathrm{d}G_{\mathrm{R}}/\mathrm{d}t$ as the instantaneous real energy $E(t)$ of the system

$$E(t) = E_0\exp(-\lambda t), E_0 = E(t=0) = W_{\mathrm{R}} - G_0\lambda. \tag{3.8}$$

$E(t)$ decays exponentially with time.

4. Schrödinger–Langevin equation: Space part

The space part satisfies (3.4). A special solution of this equation exists when

$$W_I = -\lambda\hbar/2. \tag{4.1}$$

It is given by

$$\phi = \exp[iU(x)/\hbar], \quad U(x) = B_1 + B_2 x - (mW_I/\hbar)x^2,$$
$$B_1\lambda + B_2^2/2m = W_R. \tag{4.2}$$

However, nonlinearity of SL equation does not permit the use of GBC in any simple fashion. We give below a simple perturbative scheme by expanding the separation constant W in powers of the dissipation coefficient. Put

$$W = W_0 + \eta W_1 + \eta^2 W_2 + \dots, \tag{4.3}$$

$$\phi = \phi_0 + \eta\phi_1 + \eta^2\phi_2 + \dots, \tag{4.4}$$

where the dimensionless expansion parameter η is

$$\eta \equiv \lambda\hbar/W_0, \tag{4.5}$$

and the wave functions $\phi_0, \phi_1, \phi_2, \dots$ are mutually orthogonal. The linearity of the GBC then imply that if all the ϕ_i's satisfy them so would (4.4). The various W_i's are in general complex. Using (4.3) and (4.4) in (3.4) and comparing equal powers of η we get

$$(-\hbar^2/2m)\mathrm{d}^2\phi_0/\mathrm{d}x^2 = W_0\,\phi_0, \tag{4.6}$$

$$(-\hbar^2/2m)\mathrm{d}^2\phi_1/\mathrm{d}x^2 + \frac{W_0}{2i}\ln(\phi_0/\phi_0^*)\phi_0 = W_0\phi_1 + W_1\phi_0, \tag{4.7}$$

$$-(\hbar^2/2m)\mathrm{d}^2\phi_2/\mathrm{d}x^2 + \frac{W_0}{2i}\ln\left(\frac{\phi_0}{\phi_0^*}\right)\phi_1 + \frac{W_0}{2i}\left[\frac{\phi_1}{\phi_0} - \frac{\phi_1^*}{\phi_0^*}\right]\phi_0$$
$$= W_0\phi_2 + W_1\phi_1 + W_2\phi_0. \tag{4.8}$$

We can solve these equations consecutively. Thus ϕ_0 is one of the eigenstates ψ_q of the unperturbed i.e. undamped system and W_0 the corresponding energy. The first order correction due to dissipation is then given by

$$\eta W_1 = (\lambda\hbar/2i)\frac{\int \phi_0^*\ln\left[\frac{\phi_0}{\phi_0^*}\right]\phi_0\mathrm{d}x}{\int \phi_0^*\phi_0\mathrm{d}x} \tag{4.9}$$

and

$$\phi_1 = \sum_{k\neq q} N_k\psi_k \tag{4.10}$$

with

$$N_k = -[E_q/2i(E_k - E_q)]\cdot\frac{\int \psi_k^*\ln(\psi_q/\psi_q^*)\psi_q\mathrm{d}x}{\int \psi_k^*\psi_k\mathrm{d}x}. \tag{4.11}$$

For the special case when

$$a+b=0, \quad \alpha=0, \quad \delta\neq 0 \tag{4.12}$$

the unperturbed energy eigenvalues correspond to the usual ones given by

$$\sin(kL)=0, \quad \cos(kL)=\pm 1, \quad kL=n\pi, \quad n=1,2,3,\ldots \tag{4.13}$$

Thus for ψ_0 corresponding to $k=q$, the first order correction to the energy becomes

$$\eta W_1 = \hbar\lambda \int \rho^2\Theta(x)\mathrm{d}x \Big/ \int \rho^2 \mathrm{d}x, \tag{4.14}$$

where

$$\rho^2 = \frac{q^2\cos^2(qx)+(b^2+\delta^2)\sin^2(qx)+2bq\sin(qx)\cos(qx)}{(b^2+\delta^2)} \tag{4.15}$$

and

$$\tan(\Theta) = \pm\frac{\delta q\cos(qx)}{(b^2+\delta^2)\sin(qx)+bq\cos(qx)}. \tag{4.16}$$

The upper (lower) sign corresponds to $\cos(qL)=1\,[\cos(qL)=-1]$. From (4.14) it is clear that dissipation acts in opposite directions for alternate states, one state is reduced in energy or pushed down and the other state is pulled up. Further simplification occurs when the parameter b is set equal to zero. Putting $x=L/2+y$ it is seen that the integrand is an odd function of y and the integral vanishes. Thus in this special case dissipation does not affect the energy eigenvalues to first order.

5. Results and concluding remarks

We put the dispersion relation (2.5) in dimensionless form by measuring all distances in units of Bohr radius a_0 and the wave vectors in the units of $1/a_0$, so also the parameters a, b, α and δ in the GBC. The energy E_k then becomes k^2 in Rydberg with k dimensionless for m, the electronic mass. The dependence of the eigenvalues on the size of the box, L, can be absorbed into the changed values of the parameters a, b, α, δ as shown. Multiply (2.5) by L^2 and define

$$q=kL, \alpha'=\alpha L, \delta'=\delta L, a'=aL, b'=bL$$

to cast the equation in the L independent form as

$$2q\alpha' + (a'+b')q\cos q + [a'b' - \alpha'^2 - \delta'^2 - q^2]\sin q = 0. \tag{5.1}$$

Roots of this equation correspond to k values for parameters $\alpha=\alpha'/L$ etc. The large k eigenvalues are readily seen to be the usual ones corresponding to

$$\sin q = 0 \quad \text{or} \quad q=n\pi, \quad k=n\pi/L, \quad n=1,2,3,\ldots, \tag{5.2}$$

where large k is defined by

$$k \gg |\alpha|, |\delta|, |a|, |b|. \tag{5.3}$$

When $\alpha=0$, $a+b=0$ we again have (5.2).

Another special case of interest occurs when

$$a+b=2\alpha. \tag{5.4}$$

Table 1. Ten lowest roots of the eigenvalue equation (2.5) for some values of the parameters a, b, α, δ. [The values given are in dimensionless form as explained in § 5]

Parameters for $L = 10$	Roots(kL/π)									
$a = b = \alpha = 0{\cdot}001$, $\delta = 1$	1	2	3	4	5	6	7	8	9	10
$a = b = \alpha = \delta = 1$	1	2.49	3	4.48	5	6.43	7	8.37	9	10.32
$a = 1.1, b = 0.9$, $\alpha = 1.2, \delta = 1$	0·99995	2.46	2.94	4.5	4.94	6.45	6.95	8·4	8.96	10.35

One set of eigenvalues is then given by

$$\cos(kL/2) = 0 \quad \text{or} \quad k = n\pi/L, \quad n = 1, 3, 5, \ldots, \tag{5.5}$$

corresponding to odd n values in (5.2). The other set of eigenvalues is obtained from the solutions of

$$\tan\frac{kL}{2} = \frac{2k\alpha}{\alpha^2 + \delta^2 + k^2 - ab} \tag{5.6}$$

and in general these values are shifted from the even n values of (5.2). Some numerical solutions of the eigenvalue equation (5.6) are given in table 1. It is seen that when a, b, α, δ shift from unity the odd n roots are lowered and even n values are raised thus leading to an apparent pairing of the roots.

The dispersion coefficient λ has dimensions of $1/t$. For the perturbative formulation to be applicable $1/\lambda$ should be substantially larger than the natural time scale of the problem which can be the time taken by the particle to travel from 0 to L. We thus get the condition

$$\frac{1}{\lambda} > \frac{L}{[(\hbar q/m)\mathrm{Im}(C)]}. \tag{5.7}$$

For the simple case of GBC parameter values (4.12), this reduces to

$$\lambda\hbar < \frac{2E_q\delta}{[L(b^2 + \delta^2)]}. \tag{5.8}$$

Thus the dissipation effects would be more important for low lying energy levels.

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