

Quantum Square Well Bound States Described by Equations with Non-Locality

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We present here a simple equation explicitly incorporating non-locality, which reproduces quantized energy levels of the bound states for the square well potentials. Introduction of this equation is motivated by studies of differential equation with time delayed feedback, which can be viewed as describing temporal non-locality.

KEYWORDS: non-locality, quantum mechanics, delay

1. Introduction

“Stochasticity” and “non-locality” are the two main elements, which separate quantum mechanics from classical mechanics. Probabilistic dynamics governed by the Schrödinger equation and non-local correlations as manifested by the Bell’s inequalities are representative features of quantum theory [1].

Due to these factors of stochasticity and non-locality, quantum mechanics has attracted much attention in the light of measurement theories [2, 3]. It appears that puzzles still remain (e.g., [4, 5]), and explorations, such as quantum computations and quantum information theories, are actively pursued [6].

There have been some investigations to reformulate quantum and quantum field theories with respect to the former factor of stochasticity. The main approach is to include a “noise” term explicitly in the formulation [7, 8]. However, to the author’s knowledge, analogous attempts regarding the latter factor of non-locality have not been made.

Let us first discuss what we mean by “non-locality” in this paper. We use it so as to describe effects or dynamics that involve multiple points in space and/or time, and that cannot be composed simply by combining local effects. The quantum tunneling resonance provides one such example [9, 10]. The transmission rate of two potential barriers separated spatially cannot be calculated correctly by simply “classically” combining the transmission rate of each single barrier. In fact, as is well known, total transmission could be achieved theoretically by having two potential barriers, even though each barrier is not. Thus, we need to take into account effects of non-local two points separated in space all together. The same is true temporally, as discussed by “Delayed Choice Experiments” [3, 11]. We cannot describe outcomes of such experiments by a simple combination of what is done at each local time point. Extended knowledge over time axes is needed, again, at once to understand the experimental results.

Against this background, we take the following speculative view. If it is essential to consider spatio-temporal non-local measurements or interactions to describe nature of quantum mechanics, why not take this factor at its “face value” and built it into dynamics of equation describing it? Such equation should involve multiple points of space and time variables, which we term as a “non-local” equation in this paper (as similarly as in [12, 13]).

As a first step toward this direction, we present a simple equation incorporating spatial non-locality, which gives discrete energy spectrums for quantum square well potentials. The form of this equation is motivated by considerations of non-locality on the time axes in a “classical” context, which are often described by “delay differential equations.” These equations are often used to describe dynamics under the influence of time delays as in the physiological feedbacks. Though less known in physical contexts, applications are quite wide including reproductions of blood cells, human posture balancing, neural networks, market dynamics and so on (e.g., [14]). Also, mathematically, they have been of interest as they produce rather intricate and complex dynamics to otherwise simple systems just by an increase of the value of the delay parameter [15].

The equation we present in the following is the simplest first order equation of this kind with re-interpretation of the temporal non-locality of delay as spatial non-locality. It contains only the first order derivative in space in contrast to the Schrödinger equation. Also, the boundary points of the potential are explicitly included as non-local factors “replacing” boundary conditions. With a quantization rule of imposing oscillating dynamics inside the potential well,

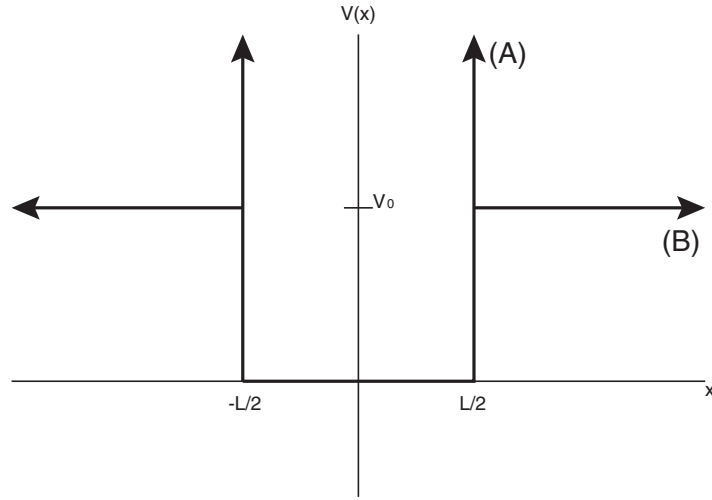


Fig. 1. Quantum square well with infinite (A) and finite (B) barrier height.

we show that it can reproduce quantized energy levels as given by the standard procedures of considering boundary conditions [16, 17].

2. Non-Local Equation

Let us start describing our equations. The first one is for the square well with infinite boundaries, as shown in Fig. 1(A). The equation is simply given as follows.

$$\frac{d\mu(x)}{dx} = \begin{cases} (i)^{1+p}k\mu(x - \frac{L}{2}), & (0 \leq x \leq \frac{L}{2}) \\ (i)^{1+p}k\mu(x + \frac{L}{2}), & (-\frac{L}{2} \leq x \leq 0) \\ 0, & (\frac{L}{2} < |x|), \end{cases} \quad (2.1)$$

where $i = \sqrt{-1}$, $k = \frac{\sqrt{2mE}}{\hbar}$ with mass, m , and energy E of the quantum particle, and $\hbar = \frac{h}{2\pi}$, h being the Plank's constant. p is a parameter which takes values 0, 1. With a step function,

$$\theta(x) = \begin{cases} +1, & (0 \leq x) \\ -1, & (x < 0), \end{cases} \quad (2.2)$$

the above equation can be written a little simpler as

$$\frac{d\mu(x)}{dx} = \begin{cases} (i)^{1+p}k\mu(x - \frac{L}{2}\theta(x)), & (|x| \leq \frac{L}{2}) \\ 0, & (\frac{L}{2} < |x|). \end{cases} \quad (2.3)$$

The quantization condition is imposing a condition that, within the well, the function $\mu(x)$ admits only the oscillatory form. Namely,

$$\mu(x) \sim e^{i\omega x}. \quad (2.4)$$

For $p = 0$, substituting this into the Eq. (2.3) yields,

$$i\omega = ik \cos\left(\frac{\omega L}{2}\right), \quad 0 = k \sin\left(\frac{\omega L}{2}\right). \quad (2.5)$$

These together leads to a quantization, $\omega^2 = k^2$ and $k_n = \frac{2n\pi}{L}$, $n = 1, 2, 3, \dots$. The associated wave function can be constructed up to the normalization constant as

$$\psi(x) \sim \begin{cases} (\mu(x) - \mu^*(x))/2 & (|x| \leq \frac{L}{2}) \\ 0 & (\frac{L}{2} < |x|). \end{cases} \quad (2.6)$$

Similarly, with $p = 1$, we obtain the other solution sets with $k_n = \frac{\pi}{L}(n + 1)$, $n = 0, 2, 4, \dots$, with the associated wave function as

$$\psi(x) \sim \begin{cases} (\mu(x) + \mu^*(x))/2 & (|x| \leq \frac{L}{2}) \\ 0 & (\frac{L}{2} < |x|). \end{cases} \quad (2.7)$$

These are well known results of the quantum bound states for this potential [18].

When the hight of potential is finite with $V_0 > E$ [Fig. 1(B)], we add a linear term in Eq. (2.3).

$$\frac{d\mu(x)}{dx} + \alpha\theta(x)\mu(x) = \begin{cases} (i)^{1+p}\gamma\mu(x - \frac{L}{2}\theta(x)) & (|x| \leq \frac{L}{2}) \\ 0 & (\frac{L}{2} < |x|), \end{cases} \quad (2.8)$$

where $\alpha = \frac{\sqrt{2m(V_0-E)}}{\hbar}$ and $\gamma = \frac{\sqrt{2mV_0}}{\hbar}$. We note an ordinary relation between these parameters, $k^2 + \alpha^2 = \gamma^2$. The θ function in the added term accounts for the finiteness of $\mu(x)$ with $x \rightarrow \pm\infty$.

By going through the same procedure of imposing the condition of Eq. (2.4), we obtain the sets of equations for $p = 0, 1$.

For $p = 0$,

$$i\omega = i\gamma \cos\left(\frac{\omega L}{2}\right), \quad \alpha = \gamma \sin\left(\frac{\omega L}{2}\right), \quad (2.9)$$

leading to $\omega^2 + \alpha^2 = \gamma^2$ and

$$\frac{\alpha L}{2} = \frac{\omega L}{2} \tan\left(\frac{\omega L}{2}\right). \quad (2.10)$$

For $p = 1$,

$$i\omega = i\gamma \sin\left(\frac{\omega L}{2}\right), \quad \alpha = -\gamma \cos\left(\frac{\omega L}{2}\right), \quad (2.11)$$

leading again to $\omega^2 + \alpha^2 = \gamma^2$, and

$$\frac{\alpha L}{2} = -\frac{\omega L}{2} \cot\left(\frac{\omega L}{2}\right). \quad (2.12)$$

By identifying $k = \omega$, Eqs. (2.10) and (2.12) give the standard quantum energy levels for this potential.

Also, the associated wave functions can be constructed, for $p = 0, 1$,

$$\psi(x) \sim \begin{cases} e^{+\alpha x} & (x < -\frac{L}{2}) \\ (\mu(x) + (-1)^p \mu^*(x))/2 & (|x| \leq \frac{L}{2}) \\ e^{-\alpha x} & (\frac{L}{2} < x). \end{cases} \quad (2.13)$$

3. Discussion

Normally, quantizations with square well potentials are done through physical considerations at the boundaries. Here, in a sense, boundaries of the potential are incorporated into the equation itself as a non-local element, and the quantization condition is given by requirements of the oscillatory nature of the solution. It is yet to be investigated whether this type of approach can be developed for obtaining or approximating quantum bound states for more general types of potentials such as a double or multiple potential barriers.

The proposed equation appears simpler as it contains only the first order derivative in space. However, in general, introduction of non-local term can give rise to quite intricate complex dynamics as shown by investigations of delay differential equations. Even though we have only focused on simple oscillatory solutions, it will be interesting to see whether some of these complex dynamical aspects of general non-local equations play roles in quantum mechanics.

Inversely, from a point of view of studies of delay differential equations, the equation here is new or not well known as it contains imaginary feedback term. Investigations of such types may reveal more interesting aspects of temporal non-locality.

In summary, this report is a modest step to speculate an alternate view on some aspects of quantum mechanics by incorporating non-locality directly into the basic equation. A question whether this style of approach can be further developed to deepen our understanding of quantum mechanics is yet to be explored.

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- [18] Note that the wave function $\psi(x)$ itself does not satisfy the differential equation. We also note that a state which is a superposition of the wave functions from the different parities does not satisfy the differential equation.
- [19] Note that combinations of the values of p and the parities of the wave functions $\psi(x)$ are different between the finite and the infinite barrier potentials.