Bound states of Newton’s equivalent finite square well

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In this paper, a 1-parameter family of Newton’s equivalent Hamiltonians (NEH) for finite square well potential is analyzed in order to obtain bound state energy spectrum and wavefunctions. For a generic potential, each of the NEH is classically equivalent to one another and to the standard Hamiltonian yielding Newton’s equations. Quantum mechanically, however, they are expected to be differed from each other. The Schrödinger’s equation coming from each of NEH with finite square well potential is an infinite order differential equation. The matching conditions therefore demand the wavefunctions to be infinitely differentiable at the well boundaries. To handle this, we provide a way to consistently truncate these conditions. It turns out as expected that bound state energy spectrum and wavefunctions are dependent on the parameter $\beta$, which is used to characterize different NEH. As $\beta \to 0$, the energy spectrum coincides with that from the standard quantum finite square well.

Keywords: Newton’s equivalent Hamiltonian; finite square well potential; bound states.

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1. Introduction

Degasperis and Ruijsenaars,1 constructed a one-parameter family of Hamiltonians whose classical version, in conservative system, is given by

$$H_\beta = \frac{1}{\beta^2 m} \left( (1 + 2m\beta^2 V(x))^{1/2} \cosh(\beta p) - 1 \right),$$

where $\beta$ is a real parameter. Each Hamiltonian in this family gives rise, via Hamilton’s equation, to the standard Newton’s equation

$$m \ddot{x} + V'(x) = 0.$$
Furthermore, in the limit $\beta \to 0$ it recovers the standard Hamiltonian, i.e.

$$\lim_{\beta \to 0} H_{\beta} = \frac{p^2}{2m} + V(x).$$

(D3)

Degasperis-Ruijsenaars construction provides one possible class of solutions to the inverse problem, which states that there can be many different Lagrangians and, as a consequence, Hamiltonians which lead the same equations of motion. For some developments in this direction, see for example Refs. 3, 4, 5, 6, 7, 8.

We will call the Hamiltonians (1) and their quantum versions as Newton’s equivalent Hamiltonians (NEH), and call the quantum theory that is based on NEH as Newton’s equivalent quantum mechanics (NEQM), while the quantum mechanics based on standard Hamiltonians will be abbreviated simply as QM.

In order to quantize each Hamiltonian (1), one inevitably faces ordering ambiguity. But instead of directly addressing the ambiguity by studying all the possible orderings, we will simply choose a particular ordering and work on it. This is also the approach adopted in Ref. 1, which studied NEH of simple harmonic oscillator by focusing on a particular operator ordering of NEH. Then after presented their result based on this particular ordering, they proceeded to discuss the results for some other orderings.

Although classically every Hamiltonian in the family describes the same theory, it is not guaranteed that quantum mechanically they would agree to each other. For example, the analysis of NEQM simple harmonic oscillator by Ref. 1 showed that although the energy spectrum (after an appropriate constant shift in the Hamiltonians) is independent of the parameter $\beta$, the wavefunctions differ from their counterpart in QM simple harmonic oscillator.

Apart from NEQM simple harmonic oscillator discussed by Ref. 1, the only other NEQM system being discussed in the literature is an NEQM plane rotator. One of the reasons that there only seem to be only a couple of NEQM analyzed so far is perhaps due to the complication of NEH in general. Schrödinger’s equations for these systems are infinite dimensional differential equations.

In this paper, we will turn our attention to NEQM finite square well. In particular, we will analyze the bound state energy levels and their corresponding wavefunctions. In the QM counterpart, the strategy to analyze the system is that one solves Schrödinger’s equation separately for the regions inside and outside of the well. Then one matches the wavefunctions on the boundaries such that they are continuous and differentiable at least once. The reason for this requirement is thanks to the fact that the Schrödinger’s equation is a second order differential equation. For NEQM case, since the Schrödinger’s equation is an infinite order differential equation, the wavefunctions have to be infinitely differentiable on the well boundaries. The full task is therefore very complicated, if not impossible to do so numerically. So we will provide a way to approximate the results and argue how the approximations are justified.

This paper is organized as follows. In Section 2 we review QM finite square well
system. We emphasize on an approach which is to be applied to the corresponding NEQM system. In Section 3 we study NEQM finite square well system for bound state case by making use of a systematic way to truncate infinitely many matching conditions at the well boundaries. The result for bound state NEQM finite square well are discussed in Section 4. We obtain the discrete energy spectrum, and explain the behavior of spectrum in this section. Finally, we conclude our work in Section 5.

2. QM finite square well

Let us give a review on QM finite square well by focusing on an approach which will be extended and applied to our analysis on NEQM finite square well to be given in later sections.

The Schrödinger’s equation for QM finite square well is given by

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) + V(x) \psi(x) = E \psi(x), \quad (4)$$

where

$$V(x) = \begin{cases} 0; & -a < x < a \\ V_0; & x < -a \ & x > a \end{cases}. \quad (5)$$

This separates the position space into three regions: Region I for $x < -a$, Region II for $-a < x < a$, and Region III for $x > a$. By demanding the wavefunction to vanish as $x \rightarrow \pm \infty$, the solution to Schrödinger’s equation at this stage is given by

$$\psi_I(x) = A e^{\kappa x}, \quad \psi_{II}(x) = B_1 \cos(kx) + B_2 \sin(kx), \quad \psi_{III}(x) = C e^{-\kappa x}, \quad (6)$$

where

$$k \equiv \sqrt{\frac{2mE}{\hbar}}, \quad \kappa \equiv \sqrt{\frac{2m(V_0 - E)}{\hbar}}, \quad (7)$$

while $\psi_I$, $\psi_{II}$, and $\psi_{III}$ are the restrictions of wavefunction to Region I, II, and III, respectively.

In order to determine the constants $A, B_1, B_2$, and $C$, one considers matching conditions at the well boundaries. At $x = -a$, these are $\psi_I(-a) = \psi_{II}(-a)$, and $\psi_I'(-a) = \psi_{II}'(-a)$. One obtains

$$A e^{-\kappa a} = B_1 \cos(ka) - B_2 \sin(ka), \quad (8)$$

$$A \kappa e^{-\kappa a} = B_1 k \sin(ka) + B_2 k \cos(ka). \quad (9)$$

At $x = a$ the matching conditions are $\psi_{III}(a) = \psi_{II}(a)$, and $\psi_{III}'(a) = \psi_{II}'(a)$. These give

$$C e^{-\kappa a} = B_1 \cos(ka) + B_2 \sin(ka), \quad (10)$$

$$- C \kappa e^{-\kappa a} = -B_1 k \sin(ka) + B_2 k \cos(ka). \quad (11)$$
Equations (8)-(11) can be rewritten in matrix form

\[
M \begin{pmatrix} A \\ B_1 \\ B_2 \\ C \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}, 
\]

(12)

where

\[
M = \begin{pmatrix} e^{-\kappa a} - \cos(ka) & \sin(ka) & 0 \\ \kappa e^{-\kappa a} - k \sin(ka) - k \cos(ka) & 0 \\ 0 & - \cos(ka) & - \sin(ka) \end{pmatrix} e^{-\kappa a}. 
\]

(13)

In order for Eq. (12) to have a non-trivial solution, we need \( \det M = 0 \). This implies

\[
2(\kappa \cos(ka) - k \sin(ka))(\kappa \sin(ka) + k \cos(ka)) = 0, 
\]

(14)

which gives

\[
\kappa = k \tan(ka), \quad \text{or} \quad \kappa = -k \cot(ka). 
\]

(15)

In order to obtain energy spectrum for bound states, these conditions are solved together with

\[
\kappa^2 + k^2 = \frac{2mV_0}{\hbar^2} 
\]

(16)

for each given \( V_0 \). The solving technique is standard and can be found in most textbooks on quantum mechanics.

Before we proceed to the case of NEQM finite square well, let us note that wavefunctions are either even or odd functions. In the case of even functions, \( B_2 = 0, C = A \), and hence

\[
M^{(e)} \begin{pmatrix} A \\ B_1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad \text{with} \quad M^{(e)} = \begin{pmatrix} e^{-\kappa a} - \cos(ka) \\ \kappa e^{-\kappa a} - k \sin(ka) - k \cos(ka) \end{pmatrix}. 
\]

(17)

For the case of odd functions, \( B_1 = 0, C = -A \), so

\[
M^{(o)} \begin{pmatrix} A \\ B_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad \text{with} \quad M^{(o)} = \begin{pmatrix} e^{-\kappa a} \sin(ka) \\ \kappa e^{-\kappa a} - k \cos(ka) \end{pmatrix}. 
\]

(18)

By using appropriate row and column operations, the matrix \( M \) can essentially be factorized as

\[
M = \begin{pmatrix} 1 & 0 & - \frac{1}{2} & 0 \\ 0 & 1 & 0 & - \frac{1}{2} \\ 1 & 0 & \frac{1}{2} & 0 \\ 0 & -1 & 0 & - \frac{1}{2} \end{pmatrix} \begin{pmatrix} M^{(e)} & 0 \\ 0 & M^{(o)} \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & \frac{1}{2} \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ 0 & 0 & -2 & 0 \end{pmatrix}, 
\]

(19)

and hence its determinant is factorized as

\[
\det M = -2 \det M^{(e)} \det M^{(o)}. 
\]

(20)

This factorization confirms that wavefunctions can only be either even or odd functions.
3. Set up for finite square well in NEQM

3.1. Schrödinger’s equation and matching conditions

Let us study NEQM finite square well, whose Hamiltonian is given by,

\[
H = \frac{1}{2\beta^2m} \left( (1 + i\beta \sqrt{2mV(x)})^{1/2} e^{-i\hbar \beta \partial_x} (1 - i\beta \sqrt{2mV(x)})^{1/2} + (i \rightarrow -i) \right) - \frac{1}{\beta^2m},
\]

(21)

where \(V(x)\) is given by Eq. (5). This potential is constant in each region. So by restricting to any particular region, we may write \(V(x) = V_c\). Then it is clear that \(V_c\) commutes with \(\partial_x\), and so can be moved to the leftmost. That is, the Schrödinger’s equation in each region can be written in the form

\[
\left( \frac{1}{2\beta^2m} (1 + \beta^2 2mV_c)^{1/2} (e^{-i\hbar \beta \partial_x} + e^{i\hbar \beta \partial_x}) - \frac{1}{\beta^2m} \right) \psi(x) = E \psi(x).
\]

(22)

Imposing an ansatz \(\psi(x) = e^{(\gamma_r + i\gamma_i)x}\), where \(\gamma_r, \gamma_i \in \mathbb{R}\), it can be seen that the values of \(\gamma_r\) and \(\gamma_i\) fall into one of the three cases, sorted by the range of validity for energy:

Case 1:

\[
\gamma_r = \frac{\pi(2n + 1)}{\hbar \beta}, \quad \gamma_i = \frac{1}{\hbar \beta} \log \left( \frac{1 + m\beta^2E}{\sqrt{1 + 2m\beta^2V_c}} \pm \sqrt{\frac{(1 + m\beta^2E)^2}{1 + 2m\beta^2V_c} - 1} \right),
\]

(23)

for \(n \in \mathbb{Z}\). This case is valid for

\[
E \leq \frac{-\sqrt{1 + 2m\beta^2V_c} - 1}{m\beta^2}.
\]

(24)

Case 2:

\[
\cos(h\beta \gamma_r) = \frac{1 + m\beta^2E}{\sqrt{1 + 2m\beta^2V_c}}, \quad \gamma_i = 0.
\]

(25)

This case is valid for

\[
\frac{-\sqrt{1 + 2m\beta^2V_c} - 1}{m\beta^2} \leq E \leq \frac{\sqrt{1 + 2m\beta^2V_c} - 1}{m\beta^2}.
\]

(26)

Case 3:

\[
\gamma_r = \frac{2n\pi}{\hbar \beta}, \quad \gamma_i = \frac{1}{\hbar \beta} \log \left( \frac{1 + m\beta^2E}{\sqrt{1 + 2m\beta^2V_c}} \pm \sqrt{\frac{(1 + m\beta^2E)^2}{1 + 2m\beta^2V_c} - 1} \right),
\]

(27)

for \(n \in \mathbb{Z}\). This case is valid for

\[
E \geq \frac{\sqrt{1 + 2m\beta^2V_c} - 1}{m\beta^2}.
\]

(28)

In the QM limit \(\beta \to 0\), case 2 applies to regions I and III, whereas case 3 applies to region II. So let us assume that this is also the case for other values of \(\beta\). Therefore, the discrete energy spectrum should fall within the range

\[
0 \leq E \leq \frac{\sqrt{1 + 2m\beta^2V_0} - 1}{m\beta^2}.
\]

(29)
The wavefunctions which satisfy regularity requirement, \( \psi(x) \to 0 \) as \( x \to \pm \infty \), are given by

\[
\psi_I(x) = \sum_{l=0}^{\infty} A_{1,l} \exp \left( \frac{2\pi lx}{\hbar \beta} \right) \exp (\rho x) + \sum_{l=1}^{\infty} A_{-1,l} \exp \left( \frac{2\pi lx}{\hbar \beta} \right) \exp (-\rho x),
\]

\[
\psi_{II}(x) = \sum_{l=-\infty}^{\infty} B_{a,l} \exp \frac{2\pi lx}{\hbar \beta} \cos(\mu x) + \sum_{l=-\infty}^{\infty} B_{b,l} \exp \frac{2\pi lx}{\hbar \beta} \sin(\mu x),
\]

\[
\psi_{III}(x) = \sum_{l=1}^{\infty} C_{1,l} \exp \left( -\frac{2\pi lx}{\hbar \beta} \right) \exp (\rho x) + \sum_{l=0}^{\infty} C_{-1,l} \exp \left( -\frac{2\pi lx}{\hbar \beta} \right) \exp (-\rho x),
\]

where

\[
\rho \equiv \frac{1}{\hbar \beta} \cos^{-1} \left( \frac{1 + m \beta^2 E}{\sqrt{1 + 2m \beta^2 V_0}} \right),
\]

\[
\mu \equiv \frac{1}{\hbar \beta} \log \left( 1 + m \beta^2 E + \sqrt{(1 + m \beta^2 E)^2 - 1} \right).
\]

The coefficients will be determined by the matching conditions at \( x = \pm a \). Since the Schrödinger’s equation (21) is a differential equation of infinite order, the wavefunction has to be differentiable infinitely many times at the boundaries \( x = \pm a \) of the well.

The matching conditions \( \psi_n^{(I)}(-a) = \psi_n^{(I)}(-a), \psi_n^{(II)}(a) = \psi_n^{(II)}(a) \) for all \( n = 0, 1, 2, \cdots \), can be translated to a matrix equation of the form

\[
M_{\infty} = \begin{pmatrix} A & \cdots & 0 \\ \vdots & \ddots & \vdots \\ B & \cdots & 0 \\ \vdots & \ddots & \vdots \\ C & \cdots & 0 \\ \vdots & \ddots & \vdots \end{pmatrix} \begin{pmatrix} 0 \\ \vdots \\ 0 \\ \vdots \end{pmatrix}.
\]

In order for the wavefunction to be nontrivial, the matrix \( M_{\infty} \) has to be singular:

\[
\det M_{\infty} = 0.
\]

The roots of this condition give the energy spectrum \( E \) for any fixed \( \beta \) and \( V_0 \). In practice, computation of determinant of \( M_{\infty} \) would require the matrix to be truncated, say to an \( N \times N \) matrix, called \( M_N \). As \( N \to \infty \), one would expect that the roots of

\[
\det M_N = 0
\]

would converge to those of Eq. (36).
3.2. A systematic truncation

Instead of arbitrarily cutting off rows and columns of $M_\infty$, let us propose a systematic way to truncate $M_\infty$. We will start from truncating the wavefunction Eqs. (30)-(32) to

$$\psi_I(x) = \sum_{l=0}^{L} A_{1,l} \exp \left( \frac{2\pi lx}{\hbar \beta} \right) \exp(\rho x) + \sum_{l=1}^{L} A_{-1,l} \exp \left( \frac{2\pi lx}{\hbar \beta} \right) \exp(-\rho x), \quad (38)$$

$$\psi_{II}(x) = \sum_{l=-L}^{L} B_{a,l} \exp \left( \frac{2\pi lx}{\hbar \beta} \right) \cos(\mu x) + \sum_{l=-L}^{L} B_{b,l} \exp \left( \frac{2\pi lx}{\hbar \beta} \right) \sin(\mu x), \quad (39)$$

$$\psi_{III}(x) = \sum_{l=1}^{L} C_{1,l} \exp \left( -\frac{2\pi lx}{\hbar \beta} \right) \exp(\rho x) + \sum_{l=0}^{L} C_{-1,l} \exp \left( -\frac{2\pi lx}{\hbar \beta} \right) \exp(-\rho x), \quad (40)$$

for $L \in \{0, 1, 2, \ldots \}$. So there are $4(2L+1)$ arbitrary constants. Furthermore, we require matching conditions to be continuous up to order $4L+1$ derivative. That is we demand

$$\psi_I^{(n)}(-a) = \psi_{II}^{(n)}(-a), \quad \psi_{III}^{(n)}(a) = \psi_{II}^{(n)}(a) \quad (41)$$

for all $n = 0, 1, 2, \ldots, 4L+1$. This gives rise to a matrix $M_{4(2L+1)}$. Then for each $\beta$ and $V_0$, we solve for the roots of $\det M_{4(2L+1)} = 0$, and study how they would converge as $L$ increases.

In fact, $\det M_{4(2L+1)}$ can be factorized as a product of determinants of matrices corresponding to even and odd wavefunctions. To show this, let us rewrite the wavefunction (38)-(40) as, note the renaming of the arbitrary constants,

$$\psi_I(x) = P(x)\vec{A}, \quad (42)$$

$$\psi_{II}(x) = Q_e(x)\vec{B}_e + Q_o(x)\vec{B}_o, \quad (43)$$

$$\psi_{III}(x) = P(-x)\vec{C}, \quad (44)$$

where $P(x), Q_e(x), Q_o(x)$ are row vectors:

$$P(x) = \left( e^{\rho x}, e^{\frac{2\pi lx}{\hbar \beta}}+\rho x, \ldots, e^{\frac{2\pi lx}{\hbar \beta}+\rho x}, \ldots, e^{\frac{2\pi lx}{\hbar \beta}-\rho x}, \ldots, e^{\frac{2\pi lx}{\hbar \beta}-\rho x} \right), \quad (45)$$

$$Q_e(x) = \left( \cos \mu x, \cosh \left( \frac{2\pi x}{\hbar \beta} \right) \cos(\mu x), \ldots, \cosh \left( \frac{2\pi lx}{\hbar \beta} \right) \cos(\mu x), \sinh \left( \frac{2\pi x}{\hbar \beta} \right) \sin(\mu x), \ldots, \sinh \left( \frac{2\pi lx}{\hbar \beta} \right) \sin(\mu x) \right), \quad (46)$$

$$Q_o(x) = \left( \sin \mu x, \cosh \left( \frac{2\pi x}{\hbar \beta} \right) \sin(\mu x), \ldots, \cosh \left( \frac{2\pi lx}{\hbar \beta} \right) \sin(\mu x), -\sinh \left( \frac{2\pi x}{\hbar \beta} \right) \cos(\mu x), \ldots, -\sinh \left( \frac{2\pi lx}{\hbar \beta} \right) \cos(\mu x) \right), \quad (47)$$
whereas $\vec{A}, \vec{B}_e, \vec{B}_o, \vec{C}$ are column vectors

$$\vec{A} = \begin{pmatrix} A_0 \\ \vdots \\ A_{2L} \end{pmatrix}, \quad \vec{B}_e = \begin{pmatrix} B_{e,0} \\ \vdots \\ B_{e,2L} \end{pmatrix}, \quad \vec{B}_o = \begin{pmatrix} B_{o,0} \\ \vdots \\ B_{o,2L} \end{pmatrix}, \quad \vec{C} = \begin{pmatrix} C_0 \\ \vdots \\ C_{2L} \end{pmatrix}. \quad (48)$$

The matching conditions then give

$$M_{4(2L+1)} \begin{pmatrix} \vec{A} \\ \vec{B}_e \\ \vec{B}_o \\ \vec{C} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad (49)$$

where

$$M_{4(2L+1)} = \begin{pmatrix} \mathcal{D}P(-a) & -\mathcal{D}Q_e(-a) & -\mathcal{D}Q_o(-a) & 0 \\ 0 & -\mathcal{D}^*Q_e(-a) & \mathcal{D}^*Q_o(-a) & \mathcal{D}^*P(-a) \end{pmatrix}. \quad (50)$$

Here we defined the operators $\mathcal{D}, \mathcal{D}^*$ such that

$$\mathcal{D}P(x) \equiv \begin{pmatrix} P(x) \\ P'(x) \\ P''(x) \\ \vdots \\ P^{(4L+1)}(x) \end{pmatrix}, \quad \mathcal{D}^*P(x) \equiv \begin{pmatrix} P(x) \\ -P'(x) \\ -P''(x) \\ \vdots \\ -P^{(4L+1)}(x) \end{pmatrix}, \quad (51)$$

and similarly for $\mathcal{D}Q_e, \mathcal{D}^*Q_e, \mathcal{D}Q_o, \mathcal{D}^*Q_o$. We have also used the identities

$$\mathcal{D}Q_e(-x) = \mathcal{D}^*Q_e(x), \quad \mathcal{D}Q_o(-x) = -\mathcal{D}^*Q_o(x). \quad (52)$$

Choosing even wavefunctions corresponds to setting $\vec{B}_o = \vec{0}, \vec{C} = \vec{A}$. So Eq. (49) becomes, after removing redundant rows,

$$M^{(e)}_{4(2L+1)} \begin{pmatrix} \vec{A} \\ \vec{B}_e \end{pmatrix} = \vec{0}, \quad \text{with} \quad M^{(e)}_{4(2L+1)} = (\mathcal{D}P(-a), -\mathcal{D}Q_e(-a)) \quad (53)$$

Similarly, choosing odd wavefunction corresponds to setting $\vec{B}_e = \vec{0}, \vec{C} = -\vec{A}$, and Eq. (49) reduces to

$$M^{(o)}_{4(2L+1)} \begin{pmatrix} \vec{A} \\ \vec{B}_o \end{pmatrix} = \vec{0}, \quad \text{with} \quad M^{(o)}_{4(2L+1)} = (\mathcal{D}P(-a), -\mathcal{D}Q_o(-a)). \quad (54)$$

After performing row and column operations, it can easily be seen that

$$\det M_{4(2L+1)} = -2 \det M^{(e)}_{4(2L+1)} \det M^{(o)}_{4(2L+1)}. \quad (55)$$
4. Results for finite square well in NEQM

Let us now discuss how to obtain bound state energy spectrum for finite square well in NEQM. For a fixed $\beta$ and $V_0$, we construct truncated matrices $M^{(e)}_{4(2L+1)}$ and $M^{(o)}_{4(2L+1)}$ by using matching conditions for even and odd wavefunctions respectively. We substitute

$$\rho = \frac{1}{\hbar \beta} \cos^{-1} \left( \frac{\cosh(h\beta \mu)}{\sqrt{1 + 2m\beta^2 V_0}} \right), \quad (56)$$

into these matrices then solve for the roots $\mu$ of $\det M^{(e)}_{4(2L+1)} = 0$ and of $\det M^{(o)}_{4(2L+1)} = 0$. They can then be used to obtained eigenstate energy from

$$E = \frac{\cosh(h\beta \mu) - 1}{m\beta^2}. \quad (57)$$

In order to do so numerically, we proceed as follows. For each $\beta$ and $V_0$, two of the $2(2L + 1) \times 2(2L + 1)$ matrices and their determinants have to be computed as functions of $\mu$. Then we make equal-spaced samplings of $\mu$ in the range

$$0 \leq \mu \leq \frac{1}{h\beta} \log \left( \sqrt{1 + 2m\beta^2 V_0} + \sqrt{2m\beta^2 V_0} \right), \quad (58)$$

and interpolate to see where $\det M^{(e)}_{4(2L+1)}$ or $\det M^{(o)}_{4(2L+1)}$ cross the horizontal axis. Then use these values of $\mu$ to obtain energy $E$.

| $L$     | $0.01$     | $1.01$     | $5.01$     | $21.01$     | $50.01$     |
|--------|------------|------------|------------|------------|------------|
| $\beta h/a$ |            |            |            |            |            |
| 0      | 1.20290    | 5.39848 $\times 10^{-1}$ | 2.45167 $\times 10^{-1}$ | 2.93025 $\times 10^{-1}$ | 5.74541 $\times 10^{-1}$ |
| 1      | 1.20028    | 5.18674 $\times 10^{-1}$ | 1.77726 $\times 10^{-1}$ | 6.87060 $\times 10^{-2}$ | 4.47974 $\times 10^{-2}$ |
| 2      | 1.19777    | 5.16123 $\times 10^{-1}$ | 1.69242 $\times 10^{-1}$ | 5.45742 $\times 10^{-2}$ | 2.93317 $\times 10^{-2}$ |
| 3      | 1.19528    | 5.15333 $\times 10^{-1}$ | 1.67528 $\times 10^{-1}$ | 5.02396 $\times 10^{-2}$ | 2.50568 $\times 10^{-2}$ |
| 4      | 1.19280    | 5.14983 $\times 10^{-1}$ | 1.66555 $\times 10^{-1}$ | 4.83072 $\times 10^{-2}$ | 2.31343 $\times 10^{-2}$ |
| 5      | 1.19035    | 5.14789 $\times 10^{-1}$ | 1.66043 $\times 10^{-1}$ | 4.72795 $\times 10^{-2}$ | 2.20836 $\times 10^{-2}$ |
| 6      | 1.18792    | 5.14665 $\times 10^{-1}$ | 1.65747 $\times 10^{-1}$ | 4.66899 $\times 10^{-2}$ | 2.14259 $\times 10^{-2}$ |
| 7      | 1.18553    | 5.14579 $\times 10^{-1}$ | 1.65559 $\times 10^{-1}$ | 4.62771 $\times 10^{-2}$ | 2.09944 $\times 10^{-2}$ |
| 8      | 1.18374    | 5.14645 $\times 10^{-1}$ | 1.65141 $\times 10^{-1}$ | 4.60012 $\times 10^{-2}$ | 2.07552 $\times 10^{-2}$ |

As $L$ increases, the result suggests that for each fixed $\beta$ and $V_0$, the energy for each state tends to converge. We demonstrate this in Tables 1-2, which show, respectively for the ground and the first excited states, energies for example value of $V_0 = 5000\hbar^2/(ma^2)$ with various $\beta$ and $L$. It can be worked out from the tables that for each fixed $\beta$, when $L$ increases the percentage difference between two consecutive values tends to decrease as $L$ increases. This is except for some cases at $L = 8$, which is probably due to some numerical difficulties. By excluding these exceptional cases,
the trend suggests that the value of energy for each fixed $\beta$ and $V_0$ should converge as $L$ increases. Furthermore for each given state, as $\beta$ is smaller, the convergence rate is quicker. For example, in Table 1 using $L = 3$ is already sufficient to obtain the ground state energy for $\beta = 1.01a/\hbar, V_0 = 5000\hbar^2/(ma^2)$, up to three significant figures. However, to obtain the same precision when $\beta = 5.01a/\hbar$, one needs $L = 8$ or beyond.

| $\beta h/a$ | $L$ | 0.01 | 0.01 | 3.01 | 5.01 | 7.01 |
|-------------|-----|------|------|------|------|------|
| 0           | 4.81188 | 3.49359 | 1.19548 $\times 10^1$ |
| 1           | 4.81122 | 3.17995 | 5.57617 |
| 2           | 4.81098 | 3.13804 | 4.83235 | 7.95547 | 1.12967 $\times 10^1$ |
| 3           | 4.81080 | 3.12516 | 4.61457 | 7.07036 | 9.61443 |
| 4           | 4.81062 | 3.11964 | 4.52332 | 6.70500 | 8.86594 |
| 5           | 4.81046 | 3.11676 | 4.47640 | 6.51993 | 8.47866 |
| 6           | 4.81030 | 3.11504 | 4.44886 | 6.41397 | 8.25470 |
| 7           | 4.81015 | 3.11391 | 4.43155 | 6.34692 | 8.11346 |
| 8           | 4.81008 | 3.11228 | 4.41955 | 6.30671 | 8.02452 |

Furthermore, there is a generic trend for the first excited state and above that in some case these states may falsely disappear for lower values of $L$, but in fact these states exist as pointed out by the result for higher values of $L$. This is demonstrated in the last two columns of Table 2.

Note that setting $L$ too high makes the size of the corresponding matrices too large, thus consuming more time in computing determinants. Furthermore, the matrices $M^{(e)}_{4(2L+1)}, M^{(o)}_{4(2L+1)}$ and their determinants need to be computed for each sample value of $\mu$. So in the data collection for the following results, we do not set the truncation parameter as high as $L = 8$, nor set the number of sample values of $\mu$ as high as 500. We will set these numbers in such a way that the computational time is tremendously reduced, and at the same time considerable precision is preserved.

In Figure 1, we show for each fixed $V_0$, the bound state energy spectrum $E$ as a function of $\beta$. A common feature is that as $\beta$ increases, states started to disappear one by one. However, it seems that ground state still exists for large values of $\beta$. We have checked that ground state exists even at $\beta = 10^6a/\hbar, V_0 = \hbar^2/(ma^2)$. The disappearance of the energy levels for states other than the ground state is due to the fact that their values grow above the upper bound $(\sqrt{1 + 2m\beta^2V_0} - 1)/(m\beta^2)$. This bound has an analogy in QM finite square well, whose bound is $V_0$, i.e. the value of $E$ cannot be larger than $V_0$. Note that consistently, $(\sqrt{1 + 2m\beta^2V_0} - 1)/(m\beta^2) \rightarrow V_0$ as $\beta \rightarrow 0$.

We also demonstrated in the figure that the spectrum for small $\beta$ converges to the spectrum for QM finite square well. This convergence justifies the $\beta \rightarrow 0$
Fig. 1. Energy level versus $\beta$ for each fixed $V_0$. From left to right and top to bottom, $ma^2V_0/\hbar^2 = 1, 50, 300, 4000$. In the data collection, we set $L = 6$ and use at least 50 sampling values of $\mu$. The crosses show the energy spectrum for QM finite square well potential.

limit. Although the result is as expected, it is not so obvious because when $L > 0$, the wavefunction Eqs. (38)-(40) contains expressions $\sim \exp(1/\beta)$, which is singular as $\beta \to 0$. For the case of $L = 0$, due to the absence of unpleasant expressions like $\sim \exp(1/\beta)$, it is easy to see that for NEQM finite square well, the limit $\beta \to 0$ indeed reduces to QM finite square well. As for $L > 0$, in order to understand these cases let us investigate the cases $L = 1, 2$ where symbolic manipulation is still tractable. We consider asymptotic expansion for $\beta \to 0$, in which $\cosh(2\pi na/(\hbar\beta)) \sim \exp(2\pi na/(\hbar\beta)), \sinh(2\pi na/(\hbar\beta)) \sim \exp(2\pi na/(\hbar\beta))$, and $\rho \sim \kappa, \mu \sim k$. The leading order of the asymptotic expansion for determinant of $M^{(c)}$ are given by

$$ \det M^{(c)}_{12} \sim \left(\frac{2\pi}{\beta \hbar}\right)^{12} 2^5 e^{-\kappa a} k \kappa (\kappa \cos(ak) - k \sin(ak)), $$

$$ \det M^{(c)}_{20} \sim \left(\frac{2\pi}{\beta \hbar}\right)^{40} 2^{22} 3^8 e^{-\kappa a} k^2 \kappa^2 (\kappa \cos(ak) - k \sin(ak)). $$

By using the relationship $M^{(c)} \to M^{(o)}$ under the transformation $\cos(a\mu) \to \sin(a\mu), \sin(a\mu) \to -\cos(a\mu)$, one can simply read off asymptotic expansion of $\det M^{(o)}_{12}, \det M^{(o)}_{20}$ by simply applying the same transformation to $\det M^{(c)}_{12}, \det M^{(c)}_{20}$, respectively. Recall that in QM finite square well, the energy levels associated to even (resp. odd) wavefunctions can be obtained from the roots of Eq. (15) with $\kappa$ given by Eq. (16), and that $k = 0$ gives a trivial wavefunction
ψ(x) = 0. So it can be concluded that asymptotically the roots of \( \det M_{4(2L+1)} = 0 \) for \( L = 1, 2 \) coincide with the ones from QM finite square well. We expect that the similar conclusions should also hold for \( L > 2 \).

In Figure 2, we show plots of \( E \) against \( \beta \) with \( ma^2V_0/\hbar^2 = 1 \) (dotted), 10 (dashed), \( 10^3 \) (dash-dot), \( 10^6 \) (solid). The results are obtained using at least 100 sample values of \( \mu \). From left to right and top to bottom, the plots are for the ground state, the first excited state, the second excited state, and the third excited state.

![Figure 2](image)

Fig. 2. Plots of \( E \) versus \( \beta \) for \( L = 6 \) with \( ma^2V_0/\hbar^2 = 1 \) (dotted), 10 (dashed), \( 10^3 \) (dash-dot), \( 10^6 \) (solid). The results are obtained using at least 100 sample values of \( \mu \). From left to right and top to bottom, the plots are for the ground state, the first excited state, the second excited state, and the third excited state.

At each fixed \( \beta \), the ground state energy seems to converge for large \( V_0 \). This can be seen in the figure that there is no noticeable difference between the cases \( V_0 = 10^3\hbar^2/(ma^2) \) (dash-dot line) and \( V_0 = 10^6\hbar^2/(ma^2) \) (solid line). The first excited state energy seems to also converge for large \( V_0 \). This can be seen in the figure that for each \( \beta \) from 0 to around \( 2a/\hbar \), there is only a slight difference of energy between the cases \( V_0 = 10^3\hbar^2/(ma^2) \) and \( V_0 = 10^6\hbar^2/(ma^2) \). The qualitative behaviors for other excited states are similar. Moreover, the higher the excited state, the smaller the range of \( \beta \) in which the energy for \( V_0 = 10^3\hbar^2/(ma^2) \) and \( V_0 = 10^6\hbar^2/(ma^2) \) agree.

After the energy levels are obtained, one can then proceed to compute wavefunctions for each level. In Table 3, we demonstrated coefficients for wavefunctions with \( \beta = 0.71a/\hbar, V_0 = 200\hbar^2/(ma^2) \), and truncation parameter \( L = 3 \). In this case, there are four energy levels. For each level, the wavefunction can be read off by substituting the coefficients using corresponding column into Eqs. (42)-(44) such that for the ground state and the second excited state, one sets \( B_{n,i} = B_i, C_{n,i} = A_i; i = 1, 2, \cdots, 7 \), whereas for the first and the third excited states, one
Table 3. Coefficients of wavefunctions for each energy level with $\beta = 0.71a/\hbar$, $V_0 = 200\hbar^2/(ma^2)$, and truncation parameter $L = 3$. Energies for states from the lowest to the highest are $6.0580 \times 10^{-1} \hbar^2/(ma^2)$, $3.0593 \hbar^2/(ma^2)$, $9.6365 \hbar^2/(ma^2)$, $2.4482 \times 10^2 \hbar^2/(ma^2)$.

|        | ground | first excited | second excited | third excited |
|--------|--------|---------------|----------------|--------------|
| $A_1 \sqrt{a}$ | $-3.8022$ | $-5.8210$ | $-5.0512$ | $1.1259$ |
| $A_2 \sqrt{a}$ | $-1.6693 \times 10^3$ | $-4.4288 \times 10^3$ | $-8.0300 \times 10^3$ | $9.8735 \times 10^3$ |
| $A_3 \sqrt{a}$ | $-6.7988 \times 10^2$ | $-1.8967 \times 10^6$ | $-3.8497 \times 10^6$ | $6.2707 \times 10^6$ |
| $A_4 \sqrt{a}$ | $-4.3605 \times 10^7$ | $-1.2960 \times 10^8$ | $-3.0768 \times 10^8$ | $7.4482 \times 10^8$ |
| $A_5 \sqrt{a}$ | $7.7739 \times 10^2$ | $2.3381 \times 10^2$ | $6.5828 \times 10^2$ | $-4.3878 \times 10^2$ |
| $A_6 \sqrt{a}$ | $4.6207 \times 10^4$ | $1.4960 \times 10^5$ | $4.6646 \times 10^5$ | $-3.2248 \times 10^5$ |
| $A_7 \sqrt{a}$ | $8.8139 \times 10^6$ | $2.8379 \times 10^7$ | $8.5620 \times 10^7$ | $-4.9321 \times 10^7$ |
| $B_1 \sqrt{a}$ | $-8.0461 \times 10^{-1}$ | $7.5687 \times 10^{-1}$ | $6.6383 \times 10^{-1}$ | $3.8105 \times 10^{-1}$ |
| $B_2 \sqrt{a}$ | $-2.5189 \times 10^{-5}$ | $2.7911 \times 10^{-5}$ | $3.0203 \times 10^{-5}$ | $2.1175 \times 10^{-5}$ |
| $B_3 \sqrt{a}$ | $-3.2560 \times 10^{-10}$ | $3.8536 \times 10^{-10}$ | $4.4497 \times 10^{-10}$ | $3.3552 \times 10^{-10}$ |
| $B_4 \sqrt{a}$ | $-9.1693 \times 10^{-16}$ | $1.1120 \times 10^{-15}$ | $1.2284 \times 10^{-15}$ | $9.1870 \times 10^{-16}$ |
| $B_5 \sqrt{a}$ | $6.5369 \times 10^{-6}$ | $-1.1918 \times 10^{-5}$ | $-1.5209 \times 10^{-5}$ | $-1.3453 \times 10^{-5}$ |
| $B_6 \sqrt{a}$ | $4.2656 \times 10^{-11}$ | $-5.9388 \times 10^{-11}$ | $-4.3040 \times 10^{-11}$ | $-3.9307 \times 10^{-11}$ |
| $B_7 \sqrt{a}$ | $-2.0909 \times 10^{-16}$ | $4.2049 \times 10^{-16}$ | $9.0814 \times 10^{-16}$ | $9.0012 \times 10^{-16}$ |

sets $B_c = 0, B_{a,i} = B_i, C_i = -A_i; i = 1, 2, \cdots, 7$.

It can be shown by direct integration that the wavefunctions obtained from Table 3 are indeed normalised. Furthermore, the matching conditions agree quite well. For example, in the case of the ground state, the values of $(\psi^{(n)}_I(-a) - \psi^{(n)}_{II}(-a))/a^n a$ for $n = 0, 1, 2, \cdots, 13$ are, respectively, $9.4792 \times 10^{-5}, -1.0214 \times 10^{-14}, 4.9794 \times 10^{-14}, 5.1514 \times 10^{-14}, 1.0258 \times 10^{-13}, 6.5654 \times 10^{-12}, -1.0525 \times 10^{-10}, -1.6844 \times 10^{-9}, -6.7354 \times 10^{-8}, -1.7243 \times 10^{-6}, -3.4485 \times 10^{-5}, -9.9325 \times 10^{-4}, -3.3547 \times 10^{-2}, -6.2158 \times 10^{-1}$. The excited states also share similar behaviors. That is, the matching conditions are satisfied quite well for $n \leq 11$, but then not so well at $n = 12, 13$.

5. Conclusion

In this work, we study NEQM finite square well systems. The analysis of these systems suggests that they are differed from the QM counterpart, though classically they describe the same dynamics. Furthermore, each of the NEQM systems are differed from each other. This is evident from the result that the energy spectrum and wavefunctions are dependent on the parameter $\beta$.

For each of these systems, the Schrödinger’s equation is an infinite order differential equation, which leads to the requirement that the wavefunctions at the well boundary has to be infinitely differentiable. In Section 4, we present a way to approximately fulfill the matching conditions. This is by truncating the wavefunctions in such a way that they still satisfy the NEQM Schrödinger’s equation but is differentiable at the well boundary only up to order $4L + 1$. Our investigation, which is demonstrated partly in Tables 1-2, suggests that the energy spectrum tend to converge. In case $\beta$ is sufficiently small, the convergence rate is already good for
small values of $L$.

NEQM finite square well systems still retain one of the qualitative results of their QM counterpart. As $V_0$ decreases, the bound states vanish one by one, leaving only the ground state when $V_0$ is sufficiently small. This is because the bound state energies cannot exceed a particular value, which depends on $V_0$. For QM finite square well, the upper bound on the bound state energy $E$ is $V_0$ itself, that is $E < V_0$. However, for NEQM finite square well, the upper bound on $E$ is now $\beta$-dependent, and is given by $\frac{\sqrt{1 + 2m\beta^2 V_0} - 1}{(m\beta^2)}$.

We have also analyzed the behavior for large $V_0$. We have found that for each fixed $\beta$, the ground state energy tends to converge for large $V_0$. This is evident in the top left of Figure 2. As for excited states, convergences also seem to be good especially for sufficiently small $\beta$.

It is a well-known fact that the $V_0 \to \infty$ limit of QM finite square well coincides with the QM infinite square well. So it is interesting to see whether this would also be the case for the NEQM case. This question is left as a possible future work.

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