PRAMANA
— journal of
physics



Vol. 70, No. 1
January 2008
pp. 27–39

# Evaluation of eigenvalues of a smooth potential via Schroedinger transmission across multi-step potential

BASUDEB SAHU[1,*], BIDHUBHUSAN SAHU[1] and SANTOSH K AGARWALLA[2]
[1]Department of Physics, North Orissa University, Baripada 757 003, India
[2]Department of Applied Physics and Ballistics, Fakir Mohan University, Balasore, India
*Corresponding author
E-mail: bd_sahu@yahoo.com; san1612@rediffmail.com

MS received 7 January 2007; revised 25 May 2007; accepted 7 August 2007

**Abstract.** In a one-dimensional quantal solution of Schroedinger equation, the general expressions for reflection and transmission coefficients are derived for a potential constituting $n$ number of rectangular wells and barriers. These expressions are readily used for the estimation of eigenvalues of a smooth potential which is simulated by a multi-step potential. The applicability of this method is demonstrated with success in potentials with different forms including the most versatile Ginocchio potential where the widely used numerical method like Runge–Kutta integration algorithm fails to yield the result. Accurate evaluation of eigenvalues free from numerical problem for any form of potentials, whether analytically solvable or not, is the highlight of the present multi-step approximation method in the theory of potential scattering.

**Keywords.** Multi-step potential; transmission across one-dimensional continuous potential; reflection and transmission coefficients.

**PACS Nos 03.65.-w; 03.65.Xp**

## 1. Introduction

The potential functions which are amenable to exact analytic quantal solutions are rare. Rarer are the instances where the one-dimensional potentials admit a simple reflection and transmission coefficient [1–4]. The question arises whether it is possible to obtain simple and easy-to-use expressions for reflection and transmission coefficients for a smoothly varying potential which is not amenable to exact analytical solutions and evaluate the correct eigenvalues which represent bound, quasi-bound, resonance states etc., generated by the potential. In this paper, we address this aspect of potential scattering in one dimension with remarkable success. A smooth potential is simulated by $n$ number of step potentials where $n$ can be infinitely large with smaller size of the steps used. For this chain of tiny step

potentials, simple expressions for reflection ($R$) and transmission ($T$) amplitudes are derived on the basis of Schroedinger transmission of particle across a potential consituting multiple rectangular wells with $n$ boundaries [5]. Using these expressions, the eigenvalues of the smooth potential are evaluated in a straightforward manner. Thus, here is a method which is partially numerical and partially analytical and it can be named multi-step approximation (MA) method for evaluation of eigenvalues of a potential in any shape. The applicability of this method is demonstrated with remarkable success in several cases of potentials including the very versatile Ginocchio potential [2]. Ginocchio potential is a peculiar potential which cannot be expressed uniformly in coordinate space as a function of distance. This feature creates a numerical problem for the use of the most popular Runge–Kutta (RK) method for this potential. In view of this, our MA method is found to be important. The straightforward and accurate evaluation of eigenvalues for any form of potential, analytically soluble or not, is the highlight of the present method in potential scattering. The generalized expression of $R$ can be slightly modified to give expression to the scattering matrix in three-dimensional study. In this paper, we present the analysis in one dimension only.

In §2, the analytical expressions for $R$ and $T$ for the rectangular chain with $n$ boundaries are presented. Section 3 contains the application to various potential forms. In §4, we summarize the results.

## 2. Formulation

We solve the Schroedinger equation in the case of a discrete quantum well potential in one dimension, which is represented in the general form as follows:

$$V(x) = \begin{cases} V_0, & x < 0, \\ V_1, & 0 \le x \le w_1, \\ V_2, & w_1 \le x \le w_1 + w_2, \\ . & \\ . & \\ V_j, & \sum_i^{j-1} w_i \le x < \sum_i^{j} w_i, \\ . & \\ . & \\ V_n, & x \ge \sum_i^{n-1} w_i. \end{cases} \tag{1}$$

Here, in the $j$th region, the strength and width of the potential are denoted by $V_j$ and $w_j$, respectively. The solution of the Schroedinger equation in the $j$th region can be expressed as

$$\psi_j(x) = a_j \mathrm{e}^{ik_j x} + b_j \mathrm{e}^{-ik_j x}, \tag{2}$$

where $j = 0, 1, 2, 3, \ldots, n$, and the wave number $k_j$ is defined as $k_j = \sqrt{\frac{2m}{\hbar^2}(E - V_j)}$ for $\sum_i^{j-1} w_i \le x \le \sum_i^{j} w_i$. Here, $E$ indicates the incident energy and $m$ stands for the mass of the particle. For completeness purpose, we may present first the results of reflection coefficient for single and double boundaries and then generalize them for $n$-boundary as given in [5]. We derive the corresponding expression for transmission coefficient in each of these situations.

### 2.1 *Single boundary potential* ($n = 1$)

In the case of a single-step potential, with the step at $x = 0$, there are two wave functions $\psi(x)$ given by (2) in the regions 0 and 1 on either side of the point $x = 0$. Matching the wave functions and the derivatives as $x = 0$ (in combination with the condition $b_1 = 0$), one gets the following set of equations:

$$a_0 + b_0 = a_1, \quad k_0 a_0 - k_0 b_0 = k_1 a_1. \tag{3}$$

These give the reflection amplitude $R$ as

$$R = r_{01} = \frac{b_0}{a_0} = \frac{k_0 - k_1}{k_0 + k_1}, \tag{4}$$

and the transmission amplitude $T$ as

$$T = \frac{a_1}{a_0} = \frac{2k_0}{k_0 + k_1}. \tag{5}$$

We can use the notation $r_{\ell j} = -r_{j\ell} = (k_\ell - k_j)/(k_\ell + k_j)$ for two neighboring regions labeled by $\ell$ and $j$.

### 2.2 *Two-boundary potential* ($n = 2$)

In the case of a two-boundary potential with boundaries at $x = 0$ and $x = w_1$, the continuity condition at boundaries along with the condition $b_2 = 0$ gives us the following set of equations:

$$\begin{aligned} &a_0 + b_0 = a_1 + b_1, \\ &k_0 a_0 - k_0 b_0 = k_1 a_1 - k_1 b_1, \end{aligned} \tag{6}$$

$$\begin{aligned} &a_1 \mathrm{e}^{ik_1 w_1} + b_1 \mathrm{e}^{-ik_1 w_1} = a_2 \mathrm{e}^{ik_2 w_1}, \\ &k_1 (a_1 \mathrm{e}^{ik_1 w_1} - b_1 \mathrm{e}^{-ik_1 w_1}) = k_2 a_2 \mathrm{e}^{ik_2 w_1}. \end{aligned} \tag{7}$$

Solving these equations we obtain the following expressions for reflection ($R$) and transmission ($T$) amplitudes:

$$R = r_{012} = \frac{b_0}{a_0} = \frac{r_{01} + r_{12} \mathrm{e}^{2ik_1 w_1}}{1 + r_{01} r_{12} \mathrm{e}^{2ik_1 w_1}}, \tag{8}$$

$$T = \frac{a_2}{a_0} = \frac{(1 + r_{01})(1 + r_{12}) \mathrm{e}^{i(k_1 - k_2) w_1}}{1 + r_{01} r_{12} \mathrm{e}^{2ik_1 w_1}}. \tag{9}$$

The corresponding coefficients for reflection and transmission are obtained by the expressions $R_c = |R|^2$ and $T_c = |T|^2$, respectively, such that $R_c + T_c = 1$.

2.3 *n-Boundary potential*

Following the above method, we can arrive at the expressions for $R$ and $T$ for $n$-boundary situation. For reflection coefficient $R_c = |R|^2$, the amplitude $R$ is given by

$$R = r_{0123\ldots n} = \frac{b_0}{a_0} = \frac{r_{01} + r_{123\ldots n}\mathrm{e}^{2ik_1w_1}}{1 + r_{01}r_{123\ldots n}\mathrm{e}^{2ik_1w_1}}. \tag{10}$$

For transmission coefficient $T_c = |T|^2$, the amplitude $T$ is given by

$$\begin{aligned} T = \frac{a_n}{a_0} &= (1 + r_{01}) \times (1 + r_{12})\mathrm{e}^{i(k_1-k_2)w_1} \\ &\times (1 + r_{23})\mathrm{e}^{i(k_2-k_3)(w_1+w_2)} \times \cdots \\ &\times (1 + r_{n-1,n})\mathrm{e}^{i(k_{n-1}-k_n)(w_1+w_2+\cdots+w_{n-1})} \\ &\times \frac{1}{1 + r_{01}r_{123\cdots n}\mathrm{e}^{2ik_1w_1}} \times \frac{1}{1 + r_{12}r_{23\cdots n}\mathrm{e}^{2ik_2w_2}} \times \cdots \\ &\times \frac{1}{1 + r_{n-2,n-1}r_{n-1,n}\mathrm{e}^{2ik_{n-1}w_{n-1}}}. \end{aligned} \tag{11}$$

In the above eqs (10) and (11), we have used

$$\begin{aligned} r_{123\cdots n} &= \frac{r_{12} + r_{23\cdots n}\mathrm{e}^{2ik_2w_2}}{1 + r_{12}r_{23\cdots n}\mathrm{e}^{2ik_2w_2}}, \\ &\vdots \\ r_{n-1,n} &= \frac{k_{n-1} - k_n}{k_{n-1} + k_n}. \end{aligned} \tag{12}$$

The recursive character of this formula is useful in the numerical evaluation of the values of $R$ and $T$. With this, we can develop a straightforward numerical program for multi-step potential for the evaluation of transmission $T_c$ and reflection $R_c$ coefficients and also the spatial variation of the wave function at a given incident energy.

In order to obtain the eigenvalues or energies of the bound states generated by an attractive potential well, the principle that is followed is to find out the energy positions of the sharp peaks in the plot of reflection coefficient $R_c = |r_{012\cdots n}|^2$ as a function of incident energy in the region $E < 0$. These discrete energies correspond to the eigenvalues that represent bound state energies of the potential. On the other hand, the minima in the variation of $R_c$ with $E$ in the region $E > 0$ correspond to eigenvalues representing metastable or resonance states.

## 3. Application

Any smoothly varying one-dimensional potential of any shape can be simulated by $n$ number of tiny steps and the above analytical expressions for $R_c$ and $T_c$ are

suitable for such multi-step potential to calculate the eigenvalues of the smooth potential under consideration. We, in this section, demonstrate the closeness of results of such representative expressions of $R_c$ and $T_c$ with the corresponding results of exact expressions in the cases of some analytically soluble potentials. The results of bound and resonance states generated by a potential which cannot be solved analytically are also estimated by our present method for illustration. To ascertain correctness and highlight the advantages, these results are compared with the results obtained by using RK method of solving Schroedinger equation.

### 3.1 *Eckart potential*

The Eckart potential is expressed as $V(x) = -(V_0/\cosh^2 \alpha x)$, where $V_0$ and $\alpha$ stand for depth and slope parameters of the potential, respectively. Such a potential is shown in figure 1 with $V_0 = 4$ fm$^{-2}$ and $\alpha = 0.7$ fm$^{-1}$. The unit of energy here is fm$^{-2}$ as we set the mass factor $2m/\hbar^2 = 1$ while solving the Schroedinger equation. For the purpose of demonstration, we, in figure 1a, show the step potential with width equal to 0.25 fm and compare the same with the Eckart potential shown as dashed curve in this figure. When the size of the step is reduced to 0.05 fm, the corresponding multi-step potential looks smooth and merges with the original potential under consideration as shown in the lower panel of figure 1b. Now for this multi-step potential with reduced step size, we use the analytical formula (10) for the reflection amplitude $R$ and hence the coefficient $R_c$ and plot the calculated results of $R_c$ as a function of energy in the range $-4$ fm$^{-2} < E < 0$ in figure 2. In this figure, the positions of the peaks correspond to energies for bound states denoted as $E_{\rm b}^{\text{multi-step}}$ and they are tabulated in the second column of table 1. As we know, the Eckart potential is exactly solvable [6] and the eigenvalues for bound states are obtained from the analytical expression

$$E_n = -\frac{\alpha^2}{4}\left\{-(1+2n) + \sqrt{1+\frac{4V_0}{\alpha^2}}\right\}^2, \tag{13}$$

where $n = 0, 1, 2, \ldots$. With the above specification of the potential parameters, the results of bound states from this formula are estimated and tabulated in the first column of table 1 as $E_{\rm b}^{\text{exact}}$. As we see, our calculated results $E_{\rm b}^{\text{multi-step}}$ are very close to these results of bound states. This potential can be solved easily for the bound state energies by the RK method. The results obtained by this method are denoted by $E_{\rm b}^{\rm RK}$ and are tabulated in the third column of table 1. By comparison it is seen that these results are also close to the corresponding exact results $E_{\rm b}^{\text{exact}}$ given in the first column. But the results $E_{\rm b}^{\text{multi-step}}$ of the present calculation look closer to the exact results $E_{\rm b}^{\text{exact}}$.

Further, we can compare the results of $R_c$ and $T_c$ as a function of positive energy calculated by our present formulation with those obtained by using exact analytical formula for the above Eckart potential in the repulsive form with a barrier of height of 4 fm$^{-2}$. In our approach, the results of $R_c$ and $T_c$ as a function of energy are obtained by using the expressions (10) and (11), respectively. On the other hand, the corresponding results are obtained from the exact formula [7] given by

**Table 1.** Energies of bound states of the attractive Eckart potential of depth 4 fm$^{-2}$ with parameters $V_0 = 4$ fm$^{-2}$ and $\alpha = 0.7$ fm$^{-1}$. $E_{\rm b}^{\rm exact}$, $E_{\rm b}^{\rm multi\text{-}step}$ and $E_{\rm b}^{\rm RK}$ represent results from eq. (13), present multi-step approximation method and Runge-Kutta method, respectively.

| $E_{\rm b}^{\rm exact}$ (fm$^{-2}$) | $E_{\rm b}^{\rm multi\text{-}step}$ (fm$^{-2}$) | $E_{\rm b}^{\rm RK}$ (fm$^{-2}$) |
|---|---|---|
| $-2.8237$ | $-2.8229$ | $-2.8240$ |
| $-0.9611$ | $-0.9612$ | $-0.9620$ |
| $-0.0782$ | $-0.0790$ | $-0.0800$ |

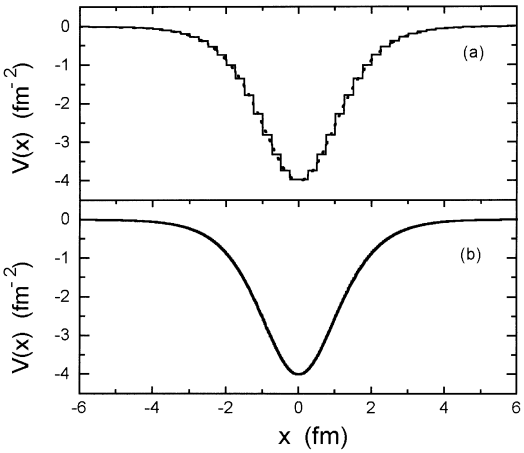


**Figure 1.** Variation of Eckart potential $V(x) = -(V_0/\cosh^2(\alpha x))$ with $V_0 = 4$ fm$^{-2}$ and $\alpha = 0.7$ fm$^{-1}$ as function of distance. (**a**) Illustration of multi-step potential with step size 0.25 fm as compared to Eckart potential (dashed curve). (**b**) Same as (**a**) but with step size 0.05 fm.

$$R_c = \frac{\cosh^2(\pi B/2)}{\sinh^2(\pi k/\alpha) + \cosh^2(\pi B/2)}, \tag{14}$$

$$T_c = \frac{\sinh^2(\pi k/\alpha)}{\sinh^2(\pi k/\alpha) + \cosh^2(\pi B/2)}, \tag{15}$$

where $B = \sqrt{(4V_0/\alpha^2) - 1}$ and $k = \sqrt{E}$. In figure 3 (upper panel), we compare our results of $R_c$ as function of energy with those of exact formula (14) and find that the two curves representing these results merge with each other. Similarly, in the lower panel of the same figure 3, the two curves representing results of $T_c$ obtained from our calculation and exact formula (15) merge with each other. Thus, we find that there is no difference between our result and that from the exact analytical formula with regard to transmission across the barrier form of Eckart potential.

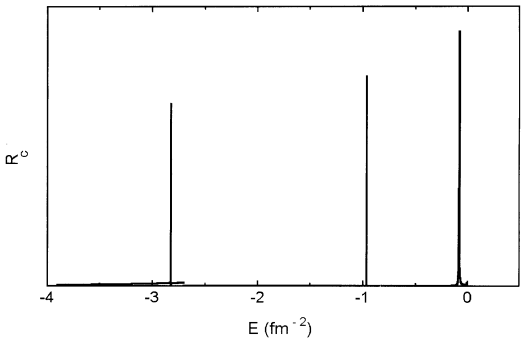


**Figure 2.** Plot of reflection coefficient $R_c$ given by (10) as a function of energy for particle in potential shown in figure 1b.

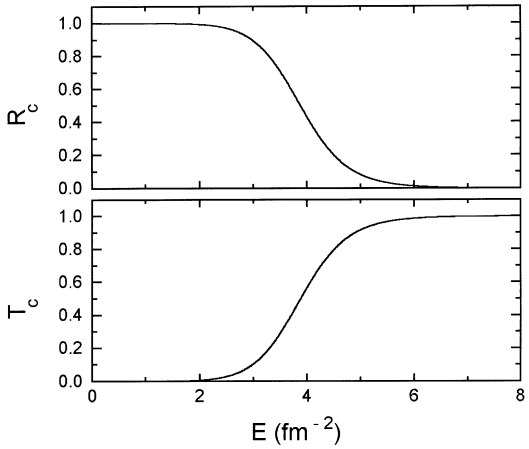


**Figure 3.** Comparison of reflection $R_c$ and transmission $T_c$ coefficients as a function of energy given by expressions (10) and (11), respectively, with the corresponding results obtained from expressions (14) and (15).

This result can be obtained by RK method with proximity. However, the present multi-step approximation method can be judged important because of the fact that it provides alternative analytical expressions for the accurate evaluation of energies of bound and resonance states for the given potential.

### 3.2 *Ginocchio potential*

Out of several solvable potential forms found in literature, the potential expressed by Ginocchio [2] in attractive form or the same potential converted to repulsive form by us in [8] finds a special place due to its flexibility to produce potentials of various shapes. It can be solved analytically for its eigenfunctions and eigenvalues. But the gray area about this potential is that in order to ascertain the computed

results from complicated analytical formulae, it is not straightforward to solve the corresponding Schroedinger equation by numerical methods, namely the most popular RK method. This is due to the nature of the above potential which cannot be expressed in coordinate space uniformly with equal intervals. As a result of this, one loses confidence in constructing any composite potential by taking different combinations of this form of potential to obtain the corresponding eigenvalues generated by the combined potential by numerical method. We use the present MA method to analyse this potential in one dimension to express the reflection coefficient as a function of energy and obtain the eigenvalues in both attractive and repulsive situations stated above.

The potential in attractive case in one dimension is given by

$$V(x) = V_0 v(r), \tag{16}$$

$$v(r) = -\lambda^2 \nu(\nu+1)(1-y^2) + \frac{1-\lambda^2}{4}[5(1-\lambda^2)y^4 - (7-\lambda^2)y^2 + 2](1-y^2). \tag{17}$$

$V_0$ is the constant potential in $\mathrm{fm}^{-2}$ unit and $r = bx$ is the dimensionless distance variable with $b = \sqrt{V_0}$. Here, $\lambda$ and $\nu$ are two dimensionless parameters. The parameter $\nu$ measures the depth of the barrier. But, when the depth at $x = 0$ denoted by $V_{0\mathrm{D}}$ is fixed it acts as a range parameter and $V_0$ is expressed accordingly in terms of $V_{0\mathrm{D}}, \lambda$ and $\nu$. The parameter $\lambda$ accounts for the flatness of the barrier. The function $y(r)$ is related to the variable $r$ by

$$r = \frac{1}{\lambda^2}[\tanh^{-1} y + (\lambda^2-1)^{1/2} \tan^{-1}(\lambda^2-1)^{1/2} y], \tag{18}$$

for $\lambda \geq 1$. With values of the parameters $\lambda = 4$ and $\nu = 5$ and depth $V_{0\mathrm{D}} = 8$ $\mathrm{fm}^{-2}$, the potential is shown in figure 4a. The analytical expression for the bound state energies is given by the formula [2]

$$E_n = V_0 \left\{ -\lambda^2 \left(\nu + \frac{1}{2}\right)^2 - (2-\lambda^2)\left(n+\frac{1}{2}\right)^2 + (2n+1)\left[\lambda^2\left(\nu+\frac{1}{2}\right)^2 + (1-\lambda^2)\left(n+\frac{1}{2}\right)^2\right]^{1/2} \right\}, \tag{19}$$

with $n = 0, 1, 2, 3, \ldots$. With the above values of the potential, the results of bound state energies designated as $E_b^{\mathrm{exact}}$ are tabulated in the first column of table 2.

As in Eckart potential case, the attractive potential shown in figure 4a is simulated by multi-step potentials with very small step size and using the expressions (10) for reflection amplitude giving the corresponding coefficient $R_c$, the results of bound states are obtained from the positions of the peaks in the plot of $R_c$ as a function of energy as shown in figure 5. These results denoted as $E_{\mathrm{b}}^{\text{multi-step}}$ are presented in the second column of table 2. A comparative analysis of our results of $E_{\mathrm{b}}^{\text{multi-step}}$ with those of $E_{\mathrm{b}}^{\mathrm{exact}}$ shows that our results are almost equal to the corresponding results estimated from the analytical formula given above.

**Table 2.** Bound state energies, $E_{\rm b}^{\rm exact}$ and $E_{\rm b}^{\rm multi\text{-}step}$, of the attractive Ginocchio potential of depth 8 fm$^{-2}$ with parameters $\lambda = 4$ and $\nu = 5$. Results of resonance state energies, $E_{nr}^{\rm zero}$ and $E_r^{\rm multi\text{-}step}$, for the same potential in repulsive form with barrier height 8 fm$^{-2}$.

| Bound state | | Resonance state | |
|---|---|---|---|
| $E_{\rm b}^{\rm exact}$ (fm$^{-2}$) | $E_{\rm b}^{\rm multi\text{-}step}$ (fm$^{-2}$) | $E_{nr}^{\rm zero}$ (fm$^{-2}$) | $E_r^{\rm multi\text{-}step}$ (fm$^{-2}$) |
| −1.307 | −1.300 | 8.668 | 8.668 |
| −3.137 | −3.137 | 9.246 | 9.246 |
| −4.885 | −4.885 | 10.403 | 10.404 |
| −6.381 | −6.381 | 12.136 | 12.135 |
| −7.525 | −7.725 | 14.448 | 14.449 |

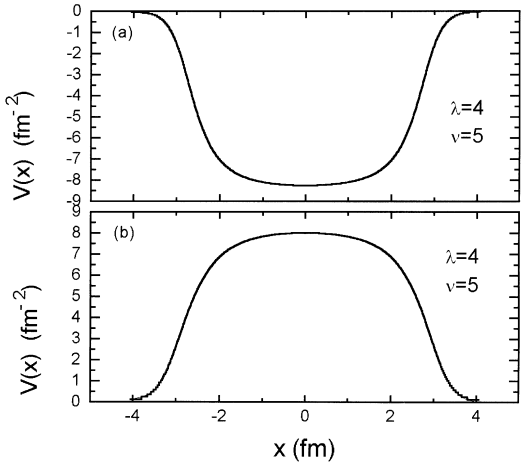


**Figure 4.** (**a**) Simulation of Ginocchio potential given by (16) with (17) by multi-step potential. Depth of the well is $V_{0\rm D} = 8$ fm$^{-2}$. (**b**) Same as (a) for potential in repulsive form given by (20). The height of the barrier is $V_{0\rm H} = 8$ fm$^{-2}$.

The Ginocchio potential given by expression (16) with (17) can be converted to repulsive situation as done in ref. [8] where the function $v(r)$ is written as

$$v(r) = \lambda^2\nu(\nu+1)(1-y^2) + \frac{1-\lambda^2}{4}[5(1-\lambda^2)y^4 - (7-\lambda^2)y^2 + 2](1-y^2). \quad (20)$$

With values of the parameters $\lambda = 4$ and $\nu = 5$ and height $V_{0\rm H} = 8$ fm$^{-2}$, the potential is shown in figure 4b. The analytical expression for transmission coefficient for this potential has been derived by us [8]. The corresponding expression for reflection coefficient can be expressed as $R_c = |R|^2$ with the reflection amplitude $R$ given by

$$R = \frac{\Gamma(ik/\lambda^2)\Gamma(1+\bar{\nu}-(ik/\lambda^2))\Gamma(-\bar{\nu}-(ik/\lambda^2))\mathrm{e}^{2ikr_1}}{\Gamma(-\bar{\nu})\Gamma(1+\bar{\nu})\Gamma(-ik/\lambda^2)}, \tag{21}$$

where

$$r_1 = \frac{1}{\lambda^2}\log\lambda - r_0,$$
$$r_0 = \frac{(\lambda^2-1)^{1/2}}{\lambda^2}\tan^{-1}(\lambda^2-1)^{1/2},$$
$$\bar{\nu} = \left\{\frac{1}{4} - \nu(\nu+1) + \frac{\lambda^2-1}{\lambda^4}k^2\right\}^{1/2} - \frac{1}{2},$$
$$k = \sqrt{\frac{E}{V_0}}.$$

For a given value of $\lambda \geq 1.4$ with some value of $\nu$ the potential can sustain resonance states in the energy region above the top of the barrier [8]. These energies are obtained from the zero of $R$ given by (21) and is represented by the formula

$$E_{nr}^{\text{zero}} = V_0\left(\frac{\lambda^4}{\lambda^2-1}\right)\left\{\left(n+\frac{1}{2}\right)^2 - \left(\frac{1}{4}-\nu^2-\nu\right)\right\}. \tag{22}$$

For a potential with barrier height $V_{0\text{H}} = 8$ fm$^{-2}$ and values of parameters $\lambda = 4$ and $\nu = 5$, the discrete results of $E_{nr}^{\text{zero}}$ near the barrier using the above formula are tabulated in the third column of table 2 under the heading 'Resonance state'. These results can also be obtained from the minima of the plot of the coefficient $R_c = |R|^2$ given by eq. (21) as a function of energy $E$. These energies situated above the barrier of height 8 fm$^{-2}$ have been named 'above barrier resonances' (ABR) in our earlier calculation [8]. We wish to verify these results now by our present MA method. The multi-step potential approximation is used for the potential shown in figure 4b and the corresponding formula for the reflection amplitude $R$ given by (10) is computed for the result of $R_c = |R|^2$ as a function of incident energy $E$. This is plotted in figure 6 and found to be oscillatory. In the same figure, we have plotted the results of $R_c = |R|^2$ obtained by using the exact analytical expression (21). As we see, the results of the present calculation completely merge with the analytical results showing no difference at any point of energy. The energy points being denoted as $E_r^{\text{multi-step}}$ corresponding to minima in this graph are collected and tabulated in the fourth column of table 2. Comparison of the respective results in columns 3 and 4 shows that our results $E_r^{\text{multi-step}}$ are almost equal to those of $E_{nr}^{\text{zero}}$ obtained by using the expression (22).

Thus, the present MA method is quite accurate in estimating eigenvalues for the Ginocchio potential in both attractive and repulsive forms. We believe that the success in reproducing exact analytical results achieved here gives one a great relief at a time when the RK approximation method of numerical calculation runs into trouble in analyzing the above important potential in the literature.

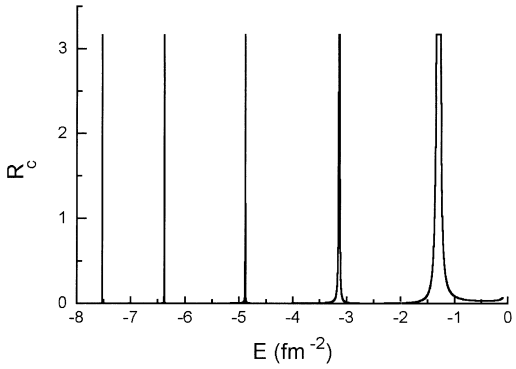


**Figure 5.** Plot of reflection coefficient $R_c$ given by (10) as a function of energy for particle in potential shown in figure 4a.

### 3.3 *Analytically not solvable potential*

In view of the remarkable success in reproducing the exact results of eigenvalues in the above two cases of potentials which are exactly solvable, we would like to mention that our present formulation is ready to provide the accurate eigenvalues representing bound, quasi-bound, resonance states etc. in any form of potential whether it is solvable or not. For illustration, we may consider the following potential which is not analytically solvable [9]:

$$V(x) = \left(\frac{1}{2}x^2 - J\right)\exp(-\lambda x^2). \tag{23}$$

With values of parameters $J = 0.55$ eV and $\lambda = 0.5$, the potential given by (23) generates an attractive well with two repulsive barriers on either side of the well as shown in figure 7. The value of the parameter $J$ decides the depth of the well at $x = 0$. As seen in figure 7, the depth of the well at the origin is $-0.55$ eV and the shoulder height of each of the two side barriers is 0.2 eV. The quantum particle considered in this potential scattering is an electron. As usual, we simulate the potential by multi-step potential and use the expression (10) to calculate the results of reflection amplitude $R$ and the corresponding coefficient $R_c$ as a function of energy ranging from $-0.55$ eV to energies more than 0.2 eV. This variation of $R_c$ with energy is shown in figure 8. In the negative energy region $E < 0$, we find two sharp peaks at energies $-0.09947$ eV and $-0.3907$ eV which represent two bound states. Further, in the same figure 8, in the positive energy region $E > 0$, the energies corresponding to the first two pointed minima of $R_c$ are recorded to be 0.1235 eV and 0.293 eV. The eigenvalue 0.1235 eV being in between $E = 0$ and 0.2 eV (shoulder height) represents a quasi-bound or metastable state whereas the eigen energy 0.293 eV in the above shoulder region would represent a resonance state. These resonance results are verified and found correct by using RK method of numerical analysis. However, in this RK method, there is difficulty in finding the bound states inside the well due to presence of thick barrier on either side of it. This difficulty is overcome in our method when we consider the part of the potential

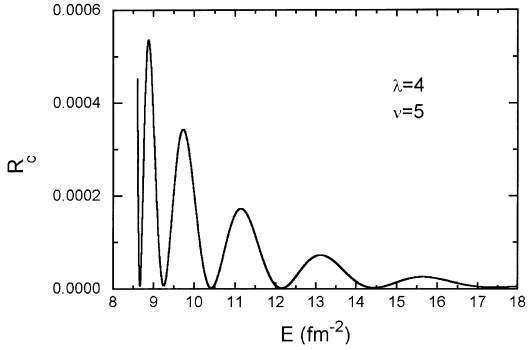


**Figure 6.** Comparison of reflection coefficient $R_c$ as a function of energy given by expression (10) with the corresponding results obtained by using analytical expression given by (21) for the particle in potential shown in figure 4b.

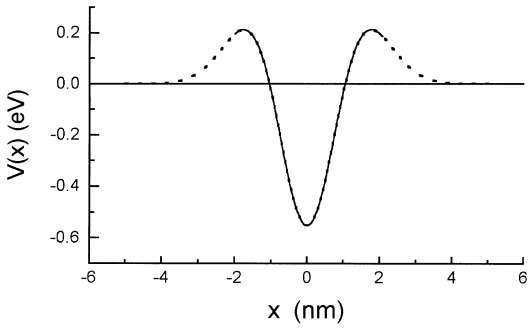


**Figure 7.** Plot of potential given by (23) as a function of distance with values of parameter $J = 0.55$ eV and $\lambda = 0.5$. The full potential is shown as dashed curve where the part covering the well region is marked by solid curve.

covering the well region only for the estimate of bound state. This reduced size of the potential is shown by a full curve in figure 7 where the tail parts on either side shown as dashed lines are not considered while estimating bound states. Such truncation of potential is not admissible in the case of RK method due to the fact that it would generate extra peak structure not representing real bound states but echoes.

## 4. Summary and conclusion

Analytical expressions for reflection ($R$) and transmission ($T$) amplitudes for a potential in one dimension consisting of multiple rectangular wells and barriers are derived. These expressions are generalized to give the results for $n$-boundary potential. Any smooth potential in one-dimensional spatial variation can be simulated or approximated by a potential consisting of $n$ number of tiny step potentials of infinitesimally small widths. The above generalized expressions of $R$ and $T$ for the

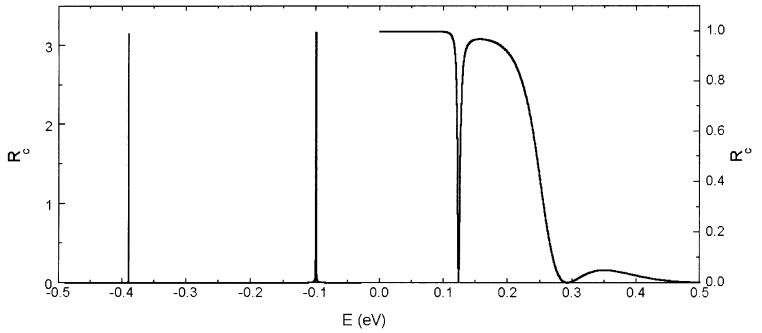


**Figure 8.** Plot of reflection coefficient $R_c$ given by (10) as a function of energy for particle in potential shown in figure 7.

$n$-boundary potential are used for this potential chain to evaluate eigenvalues of the original smooth potential. The applicability of this method is tested and found accurate in calculating bound and resonance states in some analytically soluble cases namely Eckart and Ginocchio potentials. The success in the case of Ginocchio potential is of importance due to the fact that the popular numerical method like RK method runs into trouble in analysing the results of this potential. This result would help us in a great way in studying the eigenspectra of partner potentials generated in the supersymmetric quantum mechanics of Ginocchio potential which is not yet explored exhaustively in this respect [4]. Further, the analytical formula of $n$-boundary potential can be used to reproduce very easily the well-known results of band structure of bound states for the motion of electron in a crystal as envisaged in Kronig–Penny model.

## Acknowledgement

We are thankful to Prof. C S Shastry for useful discussion. This work is supported by the Department of Science and Technology, New Delhi vide Research Grant No. SR/S2/HEP-18/2004.

## References

[1] C Eckart, *Phys. Rev.* **35**, 1303 (1930)
[2] J N Ginocchio, *Ann. Phys.* **152**, 203 (1984)
[3] Z Ahmed, *Phys. Lett.* **A157**, 1 (1991)
[4] F Cooper, A Khare and U Sukhatme, *Phys. Rep.* **251**, 267 (1995)
[5] R T Deck and Xiangshan Li, *Am. J. Phys.* **63**, 920 (1995)
[6] S Bjornholm and J E Lynn, *Rev. Mod. Phys.* **52**, 725 (1980)
[7] Z Ahmed, *Phys. Rev.* **A47**, 4761 (1993)
[8] B Sahu, S K Agarwalla and C S Shastry, *J. Phys. A: Math. Gen.* **35**, 4349 (2002)
[9] M Rittby, *Phys. Rev.* **A24**, 1636 (1981)