APPROXIMATE GROUND STATE ENERGIES OF ONE DIMENSIONAL POTENTIAL WELLS BY THE S-MATRIX FORMALISM

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ABSTRACT

APPROXIMATE GROUND STATE ENERGIES OF ONE DIMENSIONAL POTENTIAL WELLS BY THE S-MATRIX FORMALISM

One dimensional potential wells are described as a collection of consecutive thin slices, each approximated by a Dirac delta well. Bound state energies of these Dirac delta well conglomerates are calculated, using a method based on Transfer and $\mathbb{S}$-Matrix formalisms. It is observed that the method, a variant of the Born approximation, works best for the ground state energies of narrow and shallow wells. The approximate results compare favorably with the known exact results of several potential well problems.

ÖZET

BİR BOYUTLU POTANSİYEL KUYULARIN TABAN ENERJİ SEVİYELERİNE S-MATRİS YAKLAŞIMI

Bir boyutlu potansiyel kuyular önce ince dilimlere ayrılmış, sonra da bu dilimler ardışık Dirac delta kuyuları ile betimlenmiştir. Transfer ve $\mathbb{S}$ -Matrisi teorisi kullanılarak geliştirilen bir yöntemle, bu ardışık Dirac delta kuyularının bağlı durum enerjileri hesaplanmıştır. Born yaklaştırımının bir türü olan bu metodun en çok, dar ve sığ potansiyellerin taban enerjisi sonuçlarında başarılı olduğu gözlenmiştir. Elde edilen yaklaşık sonuçlar, bilinen bazı potansiyellerin kesin sonuçlarıyla karşılaştırılmış ve uyum içinde oldukları görülmüştür.

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1. INTRODUCTION

Quantum Mechanics concerns itself with the spectra and transitions between the possible states of physical systems. The idea to study scattering, the most important transition problem, by investigating the asymptotic states of particles was first conceived by Heisenberg [1, 2] . The interaction represented by a potential usually has a finite range. Outside this range, the free particle states of the incoming and outgoing particles give us information about the interaction. In this work we will first review the $\mathbb{S}$-Matrix formalism in one dimension, then concentrate on the Dirac delta potential to derive some basic results. We see the delta function as the building block of all potential profiles. This approach is analogous to slicing the inhomogeneous term of a differential equation into delta functions in Green's function approach. After obtaining the first Born approximation result using $\mathbb{S}$-Matrix techniques we will attack the bound state problem of an arbitrary well. The formalism will replace the Schrödinger differential equation by a transcendental equation. We will use this transcendental equation to solve for the ground state energies of several well known potentials and compare our results with the exact ones.

2. $\mathbb{S}$-MATRIX FORMALISM IN ONE DIMENSION

2.1. Definition of the Scattering Matrix $\mathbb{S}$

We first consider one dimensional potential functions which consists of three regions (Figure 2.1). The particle is free in the first and the third regions, while the

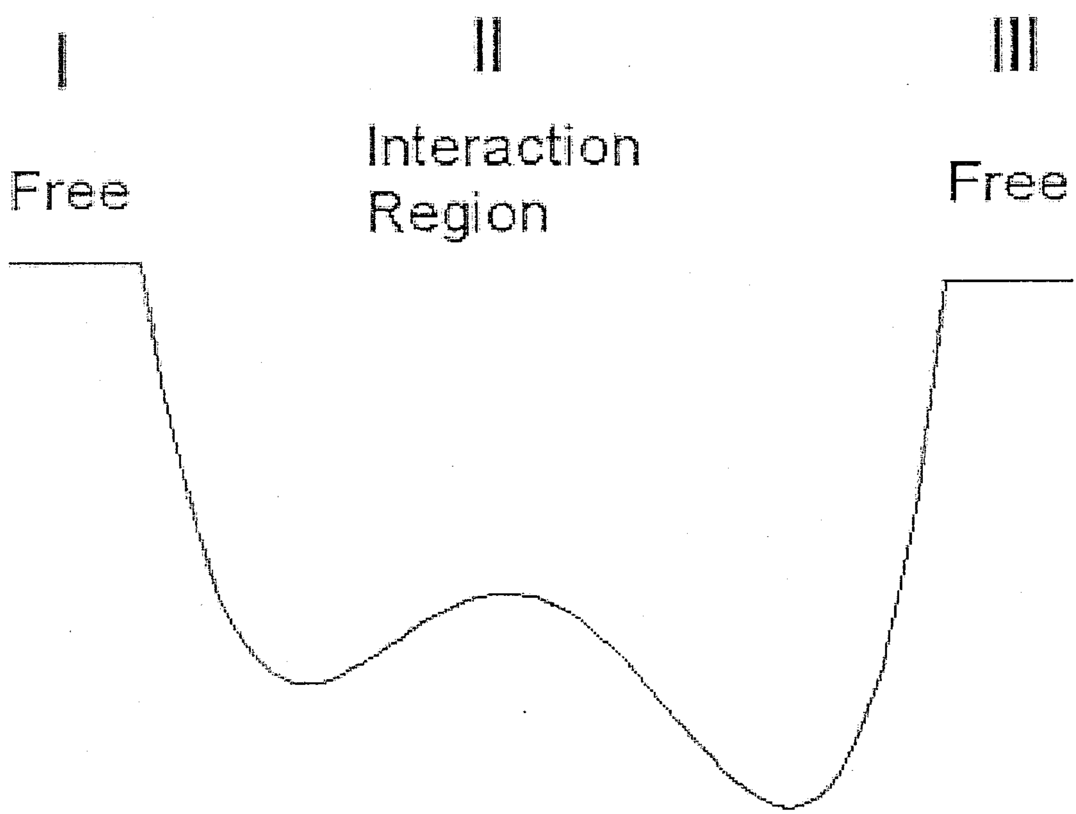

Figure 2.1. Interaction potential

second region has a non-zero potential $V(x)$. Potentials described by a single function that asymptotically goes to zero as $|x| \to \infty$ are natural candidates for this category. We proceed to solve for the wave functions by solving the one dimensional Schrödinger equation

$$\left[\frac{\hbar^2\mathbb{K}^2}{2m} + V(\mathbb{X})\right]|\Psi\rangle = \frac{\hbar^2 k_0^2}{2m}|\Psi\rangle \tag{2.1}$$

region by region. The basis of solutions for the free particle Schrödinger equation

$$\mathbb{K}^2|\Psi\rangle = k_0^2|\Psi\rangle \tag{2.2}$$

are $\{|k_0\rangle\,,\ \ |-k_0\rangle\}$. Thus the general solutions for the first and the third regions may be taken as:

$$|\psi_I\rangle = A|k_0\rangle + B|-k_0\rangle \tag{2.3}$$

$$|\psi_{III}\rangle = C|k_0\rangle + D|-k_0\rangle\ . \tag{2.4}$$

Here $A|k_0\rangle\,,\ \ D|-k_0\rangle$ are the solutions that travel towards the interaction region, while $B|-k_0\rangle\,,\ \ C|k_0\rangle$ are the solutions that move away from the interaction region. We define the $\mathbb{S}$-Matrix as a linear transformation that relates the incoming states to the outgoing states. Thus

$$\left[\ \mathbb{S}\ \right]\begin{bmatrix} A \\ D \end{bmatrix} = \begin{bmatrix} C \\ B \end{bmatrix} \tag{2.5}$$

where $\mathbb{S}$ is a two by two matrix, such that $\mathbb{S} = \mathbb{I}$ in the absence of interaction.

2.2. Definition of the Transfer Matrix $\mathbb{M}$

We may also define the transfer matrix $\mathbb{M}$ as a linear transformation relating the solutions of the two free regions:

$$\begin{bmatrix} \mathbb{M} \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} C \\ D \end{bmatrix} . \tag{2.6}$$

2.3. $\mathbb{S} = \mathbb{S}\,(m_{ij})$ and $\mathbb{M} = \mathbb{M}\,(s_{ij})$

Solving the relevant simultaneous linear equations we may write the $\mathbb{S}$-Matrix in terms of transfer matrix elements m_{ij}

$$\mathbb{S} = \frac{1}{m_{22}} \begin{bmatrix} \det(\mathbb{M}) & m_{12} \\ -m_{21} & 1 \end{bmatrix} . \tag{2.7}$$

Likewise the transfer matrix may be written in terms of $\mathbb{S}$-Matrix elements as:

$$\mathbb{M} = \frac{1}{s_{22}} \begin{bmatrix} \det(\mathbb{S}) & s_{12} \\ -s_{21} & 1 \end{bmatrix} . \tag{2.8}$$

Further, we easily see that

$$det\,(\mathbb{M}) = \frac{s_{11}}{s_{22}} \quad , \quad \det(\mathbb{S}) = \frac{m_{11}}{m_{22}} \quad , \quad m_{22} = \frac{1}{s_{22}} . \tag{2.9}$$

2.4. Transmission and Reflection Amplitudes and the S-Matrix

A one dimensional scattering experiment is essentially sending a forward wave from $x = -\infty$ and observing the reflected wave again at $x = -\infty$. We write

$$|\psi_I\rangle = |k_0\rangle + r \ |-k_0\rangle \tag{2.10}$$

$$|\psi_{III}\rangle = t \ |k_0\rangle \tag{2.11}$$

where t and r are the transmission and reflection amplitudes, respectively.
The definition of the $\mathbb{S}$-Matrix

$$\begin{bmatrix} \mathbb{S} \end{bmatrix} \begin{bmatrix} A \\ D \end{bmatrix} = \begin{bmatrix} C \\ B \end{bmatrix} \tag{2.12}$$

applied to

$$\begin{bmatrix} \mathbb{S} \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} t \\ r \end{bmatrix} \tag{2.13}$$

yields

$$\begin{bmatrix} t & ? \\ r & ? \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} t \\ r \end{bmatrix} . \tag{2.14}$$

Therefore the s_{11} and s_{21} matrix elements of the $\mathbb{S}$-matrix give the transmission and reflection amplitudes respectively.
As for the remaining two elements we consider the "reverse" scattering experiment where we send a backward wave from $x = +\infty$ and observe the reflected wave, again

at $x = +\infty$. Writing

$$|\psi_{III}\rangle = |-k_0\rangle + r' \; |k_0\rangle \tag{2.15}$$

$$|\psi_I\rangle = t' \; |-k_0\rangle \tag{2.16}$$

where we indicate the reverse reflection and transmission amplitudes by primed symbols.

$$\begin{bmatrix} \mathbb{S} \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} r' \\ t' \end{bmatrix} \tag{2.17}$$

yields the final result :

$$\mathbb{S} = \begin{bmatrix} t & r' \\ r & t' \end{bmatrix} \quad . \tag{2.18}$$

We will derive the above amplitudes later, for the specific example of a Dirac delta well. The cross section in one dimension, which is simply the reflection probability, is given by

$$P_R \equiv |r|^2 = |s_{21}|^2 \quad . \tag{2.19}$$

2.5. Bound and Virtual States From the Singularities of the $\mathbb{S}$-Matrix

When we analytically continue the $\mathbb{S}$-Matrix to complex k_0 domain, the singular points of the $\mathbb{S}$-Matrix, in other words the values of k_0 that make the $\mathbb{S}$-Matrix infinite, have special importance. Values on the imaginary axis correspond to negative energies, implying bound states. But this idea is not entirely correct; only

$Re\,(k_0) = 0,\; Im\,(k_0) > 0$ cases correspond to bound states. $Re\,(k_0) = 0,\; Im\,(k_0) < 0$ cases are called virtual states and their meaning will be explained later, in relation to the specific example of a Dirac delta well (Figure 2.2).

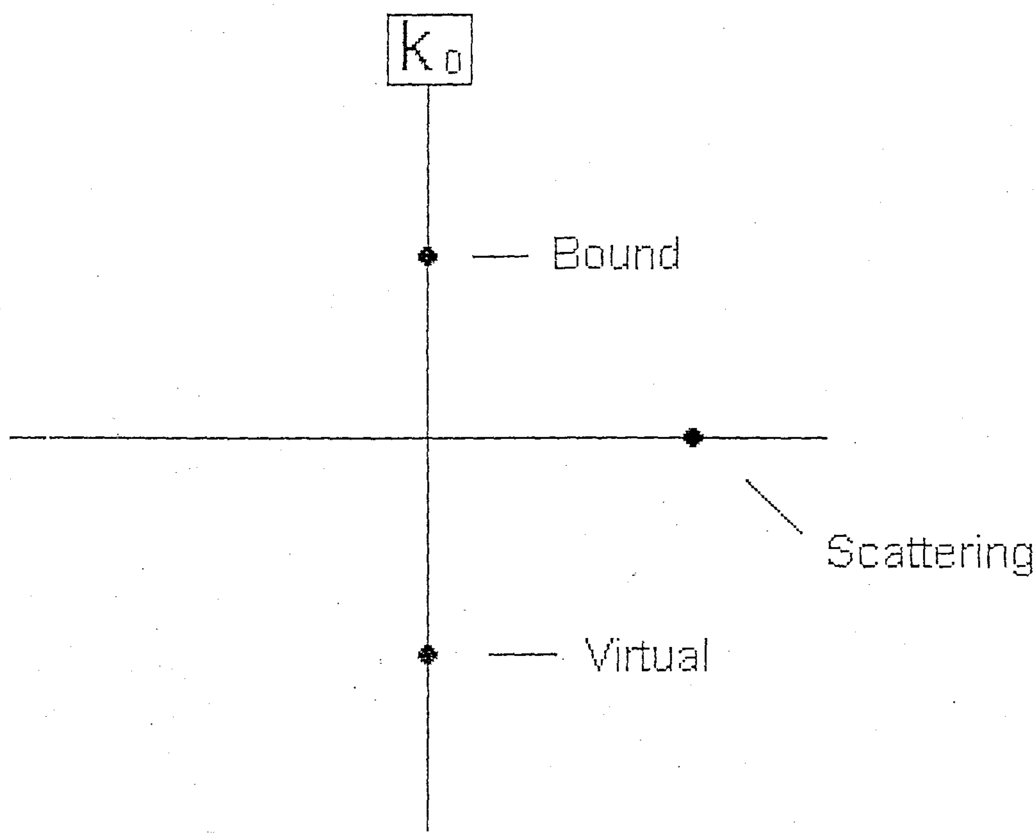

Figure 2.2. Possible singularities of the $\mathbb{S}-$ Matrix

We had expressed the $\mathbb{S}$-Matrix as

$$\mathbb{S} = \frac{1}{m_{22}} \begin{bmatrix} \det(\mathbb{M}) & m_{12} \\ -m_{21} & 1 \end{bmatrix} \tag{2.20}$$

therefore the equation $m_{22} = 0$ provides the singularities of the $\mathbb{S}$-Matrix.

2.6. Example : Dirac Delta Well

Let us consider a Dirac delta well located at $x = a$, described by the potential

$$V(x) = -\frac{\hbar^2 \sigma}{2m}\,\delta(x-a) \tag{2.21}$$

where $\sigma > 0$ [3, 4, 5]. The particle is free everywhere except for the isolated singular point at $x = a$. The wave functions which are valid in the left and right regions are

$$\Psi_L = A\frac{e^{ik_0 x}}{\sqrt{2\pi}} + B\frac{e^{-ik_0 x}}{\sqrt{2\pi}} \tag{2.22}$$

$$\Psi_R = C\frac{e^{ik_0 x}}{\sqrt{2\pi}} + D\frac{e^{-ik_0 x}}{\sqrt{2\pi}} \quad . \tag{2.23}$$

Continuity of the wave function and the discontinuity of its derivative

$$\Psi_R(a) = \Psi_L(a) \qquad ; \qquad \Psi_R^{'}(a) - \Psi_L^{'}(a) = -\sigma\Psi(a) \tag{2.24}$$

lead to equations:

$$e^{ik_0 a}\,A + e^{-ik_0 a}\,B = e^{ik_0 a}\,C + e^{-ik_0 a}\,D \tag{2.25}$$

$$\begin{aligned} &\left[ik_0\, e^{ik_0 a}\,C - ik_0\, e^{-ik_0 a}\,D\right] \quad - \quad \left[ik_0\, e^{ik_0 a}\,A - ik_0\, e^{-ik_0 a}\,B\right] = \\ &-\sigma\left[e^{ik_0 a}\,A + e^{-ik_0 a}\,B\right] \qquad . \end{aligned} \tag{2.26}$$

Now, we write these equations in matrix form as:

$$\begin{bmatrix} e^{ik_0a} & e^{-ik_0a} \\ \left(1+\frac{i\sigma}{k_0}\right)e^{ik_0a} & \left(-1+\frac{i\sigma}{k_0}\right)e^{-ik_0a} \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} e^{ik_0a} & e^{-ik_0a} \\ e^{ik_0a} & -e^{-ik_0a} \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix}, \tag{2.27}$$

so

$$\begin{bmatrix} e^{ik_0a} & e^{-ik_0a} \\ e^{ik_0a} & -e^{-ik_0a} \end{bmatrix}^{-1} \begin{bmatrix} e^{ik_0a} & e^{-ik_0a} \\ \left(1+\frac{i\sigma}{k_0}\right)e^{ik_0a} & \left(-1+\frac{i\sigma}{k_0}\right)e^{-ik_0a} \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} C \\ D \end{bmatrix}. \tag{2.28}$$

On the other hand we have defined the transfer matrix $\mathbb{M}$ as:

$$\begin{bmatrix} \mathbb{M} \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} C \\ D \end{bmatrix}. \tag{2.29}$$

Comparing the above equations we easily see that the transfer matrix $\mathbb{M}$ is given by

$$\mathbb{M} = \begin{bmatrix} 1+\frac{i\sigma}{2k_0} & \frac{i\sigma}{2k_0}e^{-2ik_0a} \\ -\frac{i\sigma}{2k_0}e^{2ik_0a} & 1-\frac{i\sigma}{2k_0} \end{bmatrix}. \tag{2.30}$$

We may also write the transfer matrix $\mathbb{M}$ as

$$\mathbb{M} = \mathbb{I} + \frac{i\sigma}{2k_0} \begin{bmatrix} 1 & e^{-2ik_0a} \\ -e^{2ik_0a} & -1 \end{bmatrix} = \mathbb{I} + \mathbb{N} \tag{2.31}$$

where $\mathbb{N}$ is a 2×2 nilpotent matrix, satisfying $\mathbb{N}^2 = 0$. Nilpotent matrices also satisfy: $Tr\,[\mathbb{N}] = 0$ and $Det\,[\mathbb{N}] = 0$.

$\mathbb{N}^2 = 0$ and $\mathbb{M} = 1 + \mathbb{N}$ imply $M = exp\,[\mathbb{N}]$, while $Tr\,[\mathbb{N}] = 0$ implies $Det\,[\mathbb{M}] = 1$. Since we plan to investigate the bound states, energies will be negative and k_0 values will have to be imaginary. Requiring the $\mathbb{S}$-Matrix to be singular, or equivalently setting $m_{22} = 0$ we indeed obtain

$$m_{22} = 1 - \frac{i\sigma}{2k_0} = 0 \;\Rightarrow\; k_0 = \frac{i\sigma}{2} \;. \tag{2.32}$$

We calculate the bound state energy eigenvalue from this equation:

$$E = \frac{\hbar^2 k_0^2}{2m} = -\frac{\hbar^2 \sigma^2}{8m} \;. \tag{2.33}$$

Note that the energy is proportional to σ^2 , so it is as if we would have a bound state even for a Dirac delta barrier: $\sigma \rightarrow -\sigma$. This unphysical bound state solution is referred to as a Virtual State. Bound and Virtual states are distinguished by their k_0 values; only $Re\,(k_0) = 0$, $Im\,(k_0) > 0$ cases are true bound states, $Re\,(k_0) = 0$ $Im\,(k_0) < 0$ cases are virtual.

By the help of the transfer matrix $\mathbb{M}$, we can construct the $\mathbb{S}$-Matrix as:

$$\mathbb{S} = \frac{1}{1 - \frac{i\sigma}{2k_0}} \begin{bmatrix} 1 & \frac{i\sigma}{2k_0} e^{-2ik_0 a} \\ \frac{i\sigma}{2k_0} e^{2ik_0 a} & 1 \end{bmatrix} \tag{2.34}$$

with

$$\det\,[\mathbb{S}] = \frac{1 + \frac{i\sigma}{2k_0}}{1 - \frac{i\sigma}{2k_0}} \;. \tag{2.35}$$

Thus the transmission amplitudes are position independent:

$$t = t' = \frac{1}{1 - \frac{i\sigma}{2k_0}} \;, \tag{2.36}$$

while the reflection amplitudes depend on the position:

$$r = \frac{\frac{i\sigma}{2k_0}}{1 - \frac{i\sigma}{2k_0}} e^{2ik_0 a} \quad , \quad r' = \frac{\frac{i\sigma}{2k_0}}{1 - \frac{i\sigma}{2k_0}} e^{-2ik_0 a} \tag{2.37}$$

where r' is simply r, but with $a \rightarrow -a$. It is worthwhile to investigate the scattering problem of the Dirac delta well using the $\mathbb{S}$-Matrix formalism. First we observe the unitarity of the $\mathbb{S}$-Matrix for real k_0

$$\mathbb{S}\,\mathbb{S}^{\dagger} = \mathbb{I} \quad \texttt{iff} \quad Im\left(k_0\right) = 0 \ . \tag{2.38}$$

Reflection amplitude $r = s_{21}$ yields

$$r = \frac{\frac{i\sigma}{2k_0} e^{2ik_0 a}}{1 - \frac{i\sigma}{2k_0}} \ . \tag{2.39}$$

Thus the cross section, or the reflection probability, becomes

$$P_R = \frac{1}{1 + \frac{4k_0^2}{\sigma^2}} \ . \tag{2.40}$$

High energy or the weak potential limit of the cross section is

$$P_{HE} \simeq \frac{\sigma^2}{4k_0^2} \ . \tag{2.41}$$

For future use, we note that the condition for the validity of this approximation is $\frac{\sigma}{2} < k_0$.

Finally let us study the double Dirac delta well described by the potential:

$$V\left(x\right) = -\frac{\hbar^2 \sigma}{2m}\left[\delta\left(x + \frac{a}{2}\right) + \delta\left(x - \frac{a}{2}\right)\right] \tag{2.42}$$

as an instructive example. In this case the overall transfer matrix is given by

$$M_T \ = \ M\left(x + \frac{a}{2}\right) M\left(x - \frac{a}{2}\right)$$

$$= \begin{bmatrix} 1+\frac{i\sigma}{2k_0} & \frac{i\sigma}{2k_0}e^{-ik_0a} \\ -\frac{i\sigma}{2k_0}e^{ik_0a} & 1-\frac{i\sigma}{2k_0} \end{bmatrix} \begin{bmatrix} 1+\frac{i\sigma}{2k_0} & \frac{i\sigma}{2k_0}e^{ik_0a} \\ -\frac{i\sigma}{2k_0}e^{-ik_0a} & 1-\frac{i\sigma}{2k_0} \end{bmatrix} .$$

Defining $k_0 \equiv i\kappa_0$; $y \equiv \kappa_0 a$, $\alpha \equiv \dfrac{\sigma a}{2}$ we get

$$M_T = \begin{bmatrix} 1+\frac{\alpha}{y} & \frac{\alpha}{y}e^{y} \\ -\frac{\alpha}{y}e^{-y} & 1-\frac{\alpha}{y} \end{bmatrix} \begin{bmatrix} 1+\frac{\alpha}{y} & \frac{\alpha}{y}e^{-y} \\ -\frac{\alpha}{y}e^{y} & 1-\frac{\alpha}{y} \end{bmatrix} \tag{2.43}$$

and then setting m_{22} equal to zero, we obtain

$$e^{-2y} = \left(1 - \frac{y}{\alpha}\right)^2 , \tag{2.44}$$

a transcendental equation, which has one or two solutions according to the value of the parameter α .

The method based on transfer matrix products is so powerful that by multiplying just two matrices, the effects of infinitely many different processes with the same outcome are covered (Appendix A). Further the formalism leads to an elegant proof of the invariance of energy spectrum under space translations (Appendix B).

3. AN APPROXIMATION METHOD FOR ARBITRARY POTENTIALS

3.1. Necessity of Approximation

It would be most convenient if it were possible to reduce all differential equations to algebraic equations. But except for very rare instances, namely linear differential equations with constant coefficients and the Euler differential equation, this is not possible. So in this study we will aim for the next best thing, reducing the Schrödinger equation to a transcendental equation, and even for that modest goal we will have to pay the price of approximating. We first consider the potential $V(x)$ consisting of successive thin slices, each slice to be approximated by a Dirac delta well (Figure 3.1).

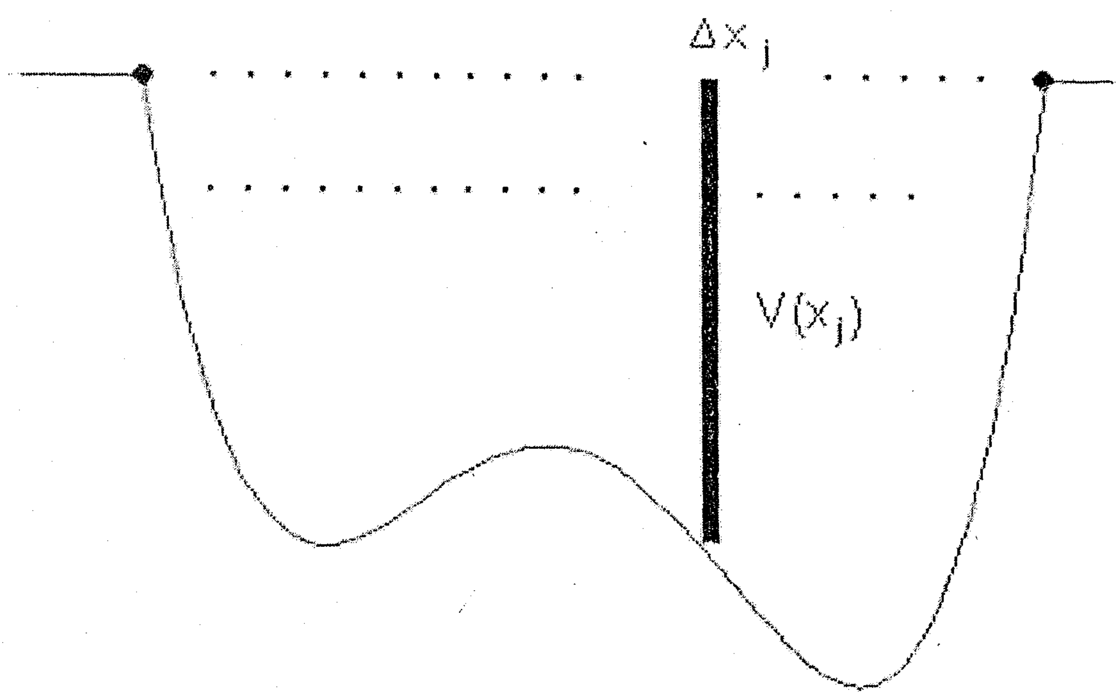

Figure 3.1. Sliced potential

Equating the areas under the potential curves we obtain the relation

$$-\frac{\hbar^2 \sigma_j}{2m} \longleftrightarrow V(x_j) \triangle x_j \tag{3.1}$$

or

$$\sigma_j \longleftrightarrow -\frac{2mV(x_j) \triangle x_j}{\hbar^2}. \tag{3.2}$$

Substituting this σ_j value into the general transfer matrix expression

$$\mathbb{M} = \mathbb{I} + \frac{i\sigma}{2k_0} \begin{bmatrix} 1 & e^{-2ik_0 a} \\ -e^{2ik_0 a} & -1 \end{bmatrix} \tag{3.3}$$

we obtain

$$\mathbb{M}_j = \mathbb{I} - \frac{im\,V(x_j) \triangle x_j}{\hbar^2 k_0} \begin{bmatrix} 1 & e^{-2ik_0 x_j} \\ -e^{2ik_0 x_j} & -1 \end{bmatrix} \tag{3.4}$$

or in exponential form as

$$\mathbb{M}_j = \exp\left(-\frac{imV(x_j) \triangle x_j}{\hbar^2 k_0} \begin{bmatrix} 1 & e^{-2ik_0 x_j} \\ -e^{2ik_0 x_j} & -1 \end{bmatrix}\right). \tag{3.5}$$

For two consecutive Dirac delta wells with

$$\mathbb{M}_1 = \exp\ (\mathbb{N}_1)\ \ and\ \ \mathbb{M}_2 = \exp(\mathbb{N}_2) \tag{3.6}$$

we cannot claim

$$\mathbb{M}_2\,\mathbb{M}_1 = \exp(\mathbb{N}_2 + \mathbb{N}_1)\quad . \tag{3.7}$$

since $\mathbb{N}_1$ and $\mathbb{N}_2$ do not necessarily commute. Therefore the product

$$exp\left(\mathbb{N}_2\right)\,exp\left(\mathbb{N}_1\right)$$

may only be approximately equal to

$$exp\left(\mathbb{N}_2 + \mathbb{N}_1\right) \quad .$$

3.2. Transfer Matrix and the Fourier Transform

We had represented the potential $V(x)$ as a succession of Dirac delta wells. For P Dirac delta wells, the overall transfer matrix $\mathbb{M}_T$ becomes

$$\mathbb{M}_T = \mathbb{M}_P \ldots \mathbb{M}_1 \simeq \exp\left[\sum_{j=1}^{P} \mathbb{N}_j\right] \quad . \tag{3.8}$$

We can write the overall transfer matrix as

$$\mathbb{M}_T \cong \exp\left(-\frac{im}{\hbar^2 k_0}\sum_{j=1}^{P} V(x_j)\,\triangle\, x_j \begin{bmatrix} 1 & e^{-2ik_0x_j} \\ -e^{2ik_0x_j} & -1 \end{bmatrix}\right) \quad . \tag{3.9}$$

Taking the limit $P \to \infty$ in the Riemann integration sense we obtain

$$\mathbb{M}_T \cong \exp\left(-\frac{im}{\hbar^2 k_0}\begin{bmatrix} \int_{-\infty}^{\infty} dx\, V(x) & \int_{-\infty}^{\infty} dx\, e^{-2ik_0x}\, V(x) \\ -\int_{-\infty}^{\infty} dx\, e^{2ik_0x}\, V(x) & -\int_{-\infty}^{\infty} dx\, V(x) \end{bmatrix}\right) \quad . \tag{3.10}$$

Remembering the Fourier transform formula

$$\tilde{V}(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx\, e^{-ikx}\, V(x) \tag{3.11}$$

the overall transfer matrix is obtained as

$$\mathbb{M}_T \cong \exp\left(-\frac{\sqrt{2\pi}im}{\hbar^2 k_0}\begin{bmatrix} \tilde{V}(0) & \tilde{V}(2k_0) \\ -\tilde{V}(-2k_0) & -\tilde{V}(0) \end{bmatrix}\right) \quad . \tag{3.12}$$

From now on we will limit ourselves only to even potentials satisfying $V(-x) = V(x)$, leading to the simplification $\tilde{V}(-2k_0) = \tilde{V}(2k_0)$. Now let us define the dimensionless quantities:

$$v = -\frac{\sqrt{2\pi} im}{\hbar^2 k_0} \tilde{V}(2k_0) = -\frac{2im}{\hbar^2 k_0} \int_0^\infty dx \cos(2k_0 x) V(x) \tag{3.13}$$

$$v_0 = -\frac{\sqrt{2\pi} im}{\hbar^2 k_0} \tilde{V}(0) = -\frac{2im}{\hbar^2 k_0} \int_0^\infty dx\, V(x) \tag{3.14}$$

for scattering, and

$$v = -\frac{2m}{\hbar^2 \kappa_0} \int_0^\infty dx \cosh(2\kappa_0 x) V(x) \tag{3.15}$$

$$v_0 = -\frac{2m}{\hbar^2 \kappa_0} \int_0^\infty dx\, V(x) \tag{3.16}$$

for bound states with $k_0 = i\kappa_0$. We observe that $v^2 \geq v_0^2$ for both cases and that

$$v_0 = \frac{1}{k_0} \lim_{k_0 \to 0} (k_0 v) = \frac{1}{\kappa_0} \lim_{\kappa_0 \to 0} (\kappa_0 v) \quad . \tag{3.17}$$

3.3. Formalism

We can write the overall transfer matrix $\mathbb{M}_T$, using only v and v_0 as:

$$\mathbb{M}_T \cong \exp \begin{bmatrix} v_0 & v \\ -v & -v_0 \end{bmatrix} \quad . \tag{3.18}$$

Rewriting $\mathbb{M}_T$ as

$$\mathbb{M}_T \cong \exp\left(\sqrt{v^2-v_0^2}\begin{bmatrix} \frac{v_0}{\sqrt{v^2-v_0^2}} & \frac{v}{\sqrt{v^2-v_0^2}} \\ -\frac{v}{\sqrt{v^2-v_0^2}} & -\frac{v_0}{\sqrt{v^2-v_0^2}} \end{bmatrix}\right) \tag{3.19}$$

and using the identity $exp\,(\gamma\Gamma) = \cos{(\gamma)}\mathbb{I} + \sin\ (\gamma)\Gamma$ where γ is an arbitrary parameter and Γ is a matrix satisfying $\Gamma^2 = -\mathbb{I}$ we obtain

$$\mathbb{M}_T = \cos\left(\sqrt{v^2-v_0^2}\right)\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + \sin\left(\sqrt{v^2-v_0^2}\right)\begin{bmatrix} \frac{v_0}{\sqrt{v^2-v_0^2}} & \frac{v}{\sqrt{v^2-v_0^2}} \\ -\frac{v}{\sqrt{v^2-v_0^2}} & -\frac{v_0}{\sqrt{v^2-v_0^2}} \end{bmatrix}. \tag{3.20}$$

3.4. First Born Approximation To Scattering

For this particular case, v and $v_0 \ll 1$ therefore the overall transfer matrix is approximately

$$\mathbb{M}_T \cong \exp\begin{bmatrix} v_0 & v \\ -v & -v_0 \end{bmatrix} \cong \begin{bmatrix} 1+v_0 & v \\ -v & 1-v_0 \end{bmatrix}. \tag{3.21}$$

Let us construct the $\mathbb{S}$-Matrix using the elements of the transfer matrix $\mathbb{M}_T$

$$\mathbb{S} \cong \begin{bmatrix} \frac{1}{1-v_0} & \frac{v}{1-v_0} \\ \frac{v}{1-v_0} & \frac{1}{1-v_0} \end{bmatrix}. \tag{3.22}$$

We can easily identify the reflection amplitude as

$$r = s_{21} \simeq \frac{v}{1-v_0} \simeq v \tag{3.23}$$

by observing the $\mathbb{S}$-Matrix, so

$$r \cong v = -\frac{\sqrt{2\pi}im}{\hbar^2 k_0}\tilde{V}\left(-2k_0\right), \tag{3.24}$$

and the cross section (reflection probability) is given by

$$P_R = \frac{2\pi m^2}{\hbar^4 k_0^2} \left| \tilde{V} \left(-2k_0 \right) \right|^2 \tag{3.25}$$

which is the well known first Born approximation result (Appendix C).

3.5. First Born Approximation To Bound States

We had seen that the positive imaginary singularities of the $\mathbb{S}$-Matrix yield bound states, and the singularities of the $\mathbb{S}$-Matrix are obtained from the equation $m_{22} = 0$. We use the above expression for $\mathbb{M}_T$ and obtain the transcendental equation

$$\tan\left(\sqrt{v^2 - v_0^2}\right) = \frac{\sqrt{v^2 - v_0^2}}{v_0} \tag{3.26}$$

or the more convenient

$$\cos\left(\sqrt{v^2 - v_0^2}\right) = \frac{v_0}{v} \tag{3.27}$$

where

$$\begin{aligned} v &= -\frac{2m}{\hbar^2 \kappa_0} \int_0^\infty dx \, \cosh\left(2\kappa_0 x\right) \, V\left(x\right) \\ v_0 &= -\frac{2m}{\hbar^2 \kappa_0} \int_0^\infty dx \, V\left(x\right) \end{aligned}$$

To check the self consistency of the above method, let us consider the Dirac delta well $V\left(x\right) = -\dfrac{\hbar^2 \sigma}{2m} \delta\left(x\right)$ which gives $v = v_0 = \dfrac{\sigma}{2\kappa_0}$. Since the argument of the tangent function in $\tan\left(\sqrt{v^2 - v_0^2}\right) = \dfrac{\sqrt{v^2 - v_0^2}}{v_0}$ is practically zero the $\sqrt{v^2 - v_0^2}$ terms cancel to yield $v_0 = \dfrac{\sigma}{2\kappa_0} = 1 \;\Rightarrow\; \kappa_0 = \dfrac{\sigma}{2}$ and the familiar $E = -\dfrac{\hbar^2 \sigma^2}{8m}$ is obtained.

4. APPLICATION I : PERIODICAL DIRAC DELTA WELLS

4.1. General Formalism

Let us consider an interaction composed of $P = 2N + 1$ equidistant identical Dirac delta wells represented by the potential:

$$V(x) = -\frac{\hbar^2 \sigma}{2m} \sum_{n=-N}^{N} \delta(x - na) \quad . \tag{4.1}$$

At first sight it seems that this analysis is limited only to an odd number of wells, but by allowing N, therefore n to take half integer values, even P values are also covered. We had defined

$$v \equiv -\frac{m}{\hbar^2 \kappa_0} \int_{-\infty}^{\infty} dx\, e^{2\kappa_0 x}\, V(x) \quad . \tag{4.2}$$

Substituting $V(x)$ into this definition we obtain

$$v = \frac{\sigma}{2\kappa_0} \frac{\sinh(P\kappa_0 a)}{\sinh(\kappa_0 a)} \tag{4.3}$$

for the derivation of this equation look at the Appendix. Using the formula

$$v_0 = \frac{1}{\kappa_0} \lim_{\kappa_0 \to 0} (\kappa_0 v) \tag{4.4}$$

we obtain

$$v_0 = \frac{\sigma P}{2\kappa_0} \quad . \tag{4.5}$$

Defining $y \equiv \kappa_0 a$, $\alpha \equiv \frac{\sigma a}{2}$ the transcendental equation

$$\tan\left(\sqrt{v^2 - v_0^2}\right) = \frac{\sqrt{v^2 - v_0^2}}{v_0} \tag{4.6}$$

becomes

$$\tan\left[\frac{\alpha P}{y}\sqrt{\frac{\sinh^2\,(Py)}{P^2\sinh^2\,(y)} - 1}\right] = \sqrt{\frac{\sinh^2\,(Py)}{P^2\sinh^2\,(y)} - 1}\ . \tag{4.7}$$

4.2. P=2 Special Case : Double Delta Well

To investigate the double delta well problem we set $P = 2$ in the above equation to obtain

$$v = \frac{2\alpha}{y}\cosh(y) \quad , \quad v_0 = \frac{2\alpha}{y} \tag{4.8}$$

$$\tan\left[2\alpha\frac{\sinh\,(y)}{y}\right] = \sinh(y) \tag{4.9}$$

or its alternate version:

$$\cos\left[2\alpha\frac{\sinh\,(y)}{y}\right] = \frac{1}{\cosh(y)}\ . \tag{4.10}$$

The transcendental equation for the exact result was shown to be:

$$\exp\,(-2y) = \left(1 - \frac{y}{\alpha}\right)^2\ . \tag{4.11}$$

Making the correct choice for sign, we obtain the equation that yields the ground state energy:

$$\exp\,(-y) = -1 + \frac{y}{\alpha}\ . \tag{4.12}$$

Table 4.1. Double Delta

α	y_{exact}	y_{Born}	error
0.001	0.001998	0.002	0.20 %
0.002	0.003999203	0.004	0.40 %
0.005	0.00995049	0.001	1.00 %
0.01	0.0198039	0.020003	2.02 %
0.02	0.0392306	0.040021	4.07 %
0.05	0.0954483	0.100336	10.50 %.
0.1	0.183255	0.202748	22.41 %
0.2	0.342061	0.424297	53.86 %
0.5	0.738835	1.00824	86.22 %

It is worth noting that both the exact and the first Born approximation equations yield $y = 2\alpha$ as $\alpha \to 0$. This is in accordance with the expected

$$\kappa_0 = \sigma \;\rightarrow\; E = -\frac{\hbar^2 \sigma^2}{2m} \tag{4.13}$$

result. The values of y, both exact and approximate, for different values of α are presented below in Table 4.1 .

The approximation error

$$\epsilon = \left| \frac{E_{exact} - E_{Born}}{E_{exact}} \right| \tag{4.14}$$

reduces to

$$\epsilon = \left| 1 - \left(\frac{y_{Born}}{y_{exact}} \right)^2 \right| \tag{4.15}$$

since $E \sim y^2$. These values are consistent with the series solution for y, obtained by analytical methods. Only the first two terms were kept for y_{exact} and y_{Born} , while one term was sufficient for % Error.

$$y_{exact} = 2\alpha - 2\alpha^2 + \ldots \tag{4.16}$$

$$y_{Born} = 2\alpha + \frac{8}{3}\alpha^3 + \ldots \tag{4.17}$$

$$\%\, error \cong 200\,\alpha\,\% \ . \tag{4.18}$$

The graph of % error plotted against $\log(\alpha)$ is presented in Figure 4.1 .

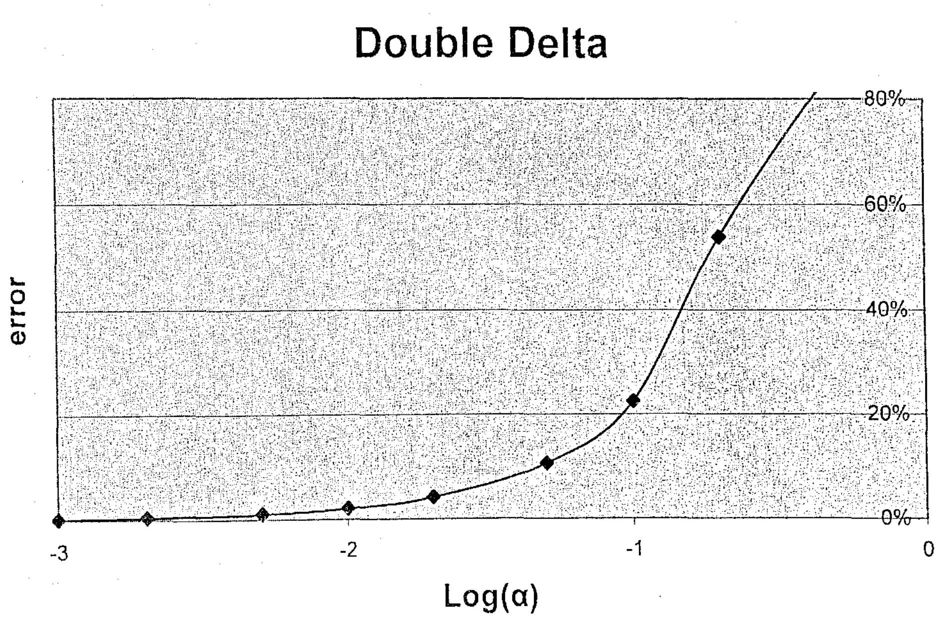

Figure 4.1. % Error vs. log (α) for Double Delta

5. APPLICATION II : FINITE SQUARE WELL

5.1. Parametrization

Before proceeding with the standard square well problem:

$$V(x) = \begin{cases} -V_0 & , \quad |x| < \frac{a}{2} \\ 0 & , \quad |x| > \frac{a}{2} \end{cases} \tag{5.1}$$

we reparametrize $V(x)$ such that $-V_0 a$, the area under the potential curve equals to the area under a Dirac delta well:

$$V(x) = -\frac{\hbar^2 \sigma}{2m} \, \delta(x) \quad . \tag{5.2}$$

Equating $-V_0 a = -\frac{\hbar^2 \sigma}{2m}$ we replace V_0 by $\frac{\hbar^2 \sigma}{2ma}$ and use the potential

$$V(x) = \begin{cases} -\frac{\hbar^2 \sigma}{2ma} & , \quad |x| < \frac{a}{2} \\ 0 & , \quad |x| > \frac{a}{2} \end{cases} \quad . \tag{5.3}$$

5.2. Exact Result

The transcendental equation for the exact ground state energy of a finite square well, one of the classic problems of quantum mechanics, is known to be,

$$\tan\left[\frac{1}{2}\sqrt{2\alpha - y^2}\right] = \frac{y}{\sqrt{2\alpha - y^2}} \qquad [6] \tag{5.4}$$

where $y \equiv \kappa_0 a$, $\alpha \equiv \frac{\sigma a}{2}$ and $E = -\frac{\hbar^2 y^2}{2ma^2}$.

Table 5.1. Square Well

α	y_{exact}	y_{Born}	error
0.001	0.000999667	0.001	0.07 %
0.002	0.00199867	0.002	0.13 %
0.005	0.00499169	0.005	0.33 %
0.01	0.00996687	0.01	0.67 %
0.02	0.0198683	0.020001	1.34 %
0.05	0.0491908	0.050014	3.37 %
0.1	0.09685532	0.100111	6.84 %
0.2	0.188065	0.200899	14.11 %
0.5	0.435131	0.514904	40.03 %

5.3. Born Approximation

Using the familiar formula for v , we obtain

$$v = \frac{\sigma}{\kappa_0 a} \int_0^{\frac{a}{2}} dx \cosh(2\kappa_0 x) = \frac{\sigma}{2\kappa_0^2 a} \sinh(\kappa_0 a) = \frac{\alpha}{y^2} \sinh(y) \tag{5.5}$$

and the limiting procedure yields $v_0 = \frac{\alpha}{y}$. Thus the transcendental equation for the Born approximation becomes:

$$\tan\left[\frac{\alpha}{y}\sqrt{\frac{\sinh^2(y)}{y^2} - 1}\right] = \sqrt{\frac{\sinh^2(y)}{y^2} - 1} \quad . \tag{5.6}$$

5.4. Error Analysis

The values of y, both exact and approximate, for different values of α are presented below in Table 5.1. The approximation error is given by

$$\left(\frac{y_{Born}}{y_{exact}}\right)^2 - 1 \tag{5.7}$$

since $E \sim y^2$. These values are consistent with the series solutions for y, obtained by analytical methods. Only the first two terms were kept for y_{exact} and y_{Born}, while one term was sufficient for % Error.

$$y_{exact} = \alpha - \frac{\alpha^2}{3} + \dots \tag{5.8}$$

$$y_{Born} = \alpha + \frac{\alpha^3}{9} + \dots \tag{5.9}$$

$$\%Error \cong \frac{200\alpha}{3}\ \% \ . \tag{5.10}$$

The graph of % error plotted against log (α) is presented in Figure 5.1 .

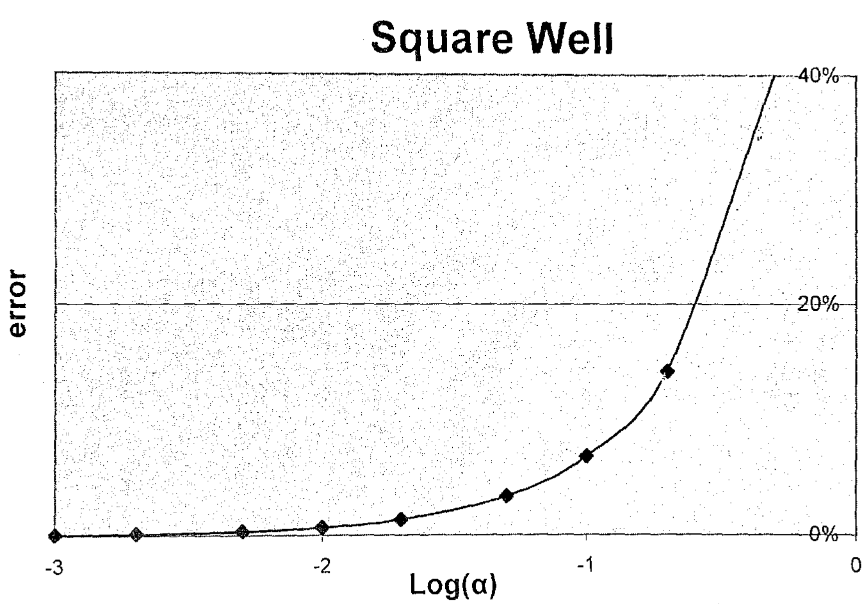

Figure 5.1. % error vs. log(α)for finite square well

6. APPLICATION III : PÖSCHL-TELLER POTENTIAL

6.1. Parametrization

Before proceeding with the Pöschl - Teller problem:

$$V(x) = -\frac{V_0}{\cosh^2(bx)} \tag{6.1}$$

we reparametrize b, the width of the potential $V(x)$ as $b = \frac{\pi}{a}$ and, its strength such that $-\frac{2aV_0}{\pi}$, and the area under the potential curve equals to the area under the Dirac delta well

$$V(x) = -\frac{\hbar^2\sigma}{2m}\,\delta(x) \ . \tag{6.2}$$

Equating $-\frac{2aV_0}{\pi} = -\frac{\hbar^2\sigma}{2m}$ we replace V_0 by $\frac{\pi\hbar^2\sigma}{4ma}$ and use the potential

$$V(x) = -\frac{\pi\hbar^2\sigma}{4ma\cosh^2\left(\frac{\pi x}{a}\right)} \ . \tag{6.3}$$

6.2. Exact Result

The Pöschl-Teller potential is one of the few quantum mechanics problems that are exactly solvable. The exact ground state energy is given by

$$E_0 = \frac{\pi^2\hbar^2}{2ma^2}\left[\sqrt{\frac{1}{4}+\frac{\sigma a}{2\pi}}-\frac{1}{2}\right]^2 \ . \tag{6.4}$$

This corresponds to $y = \pi\left[\sqrt{\frac{1}{4}+\frac{\alpha}{\pi}}-\frac{1}{2}\right]$ using $y \equiv \kappa_0 a$, $\alpha \equiv \frac{\sigma a}{2} = \frac{\pi\sigma}{2b}$, $E = -\frac{\hbar^2\kappa_0^2}{2m}$.

Table 6.1. Pöschl-Teller

α	y_{exact}	y_{Born}	error
0.001	0.000999682	0.001	0.06 %
0.002	0.0199873	0.002	0.13 %
0.005	0.00499207	0.005	0.32 %
0.01	0.00996837	0.01	0.64 %
0.02	0.0198743	0.020001	1.28 %
0.05	0.0492286	0.050014	3.22 %
0.1	0.0970047	0.100112	6.51 %
0.2	0.188669	0.200901	13.39 %
0.5	0.43873	0.515193	37.89 %

6.3. Born Approximation

Using the familiar formula for v, we obtain

$$v = \frac{\alpha}{\sin(y)} \tag{6.5}$$

and the limiting procedure yields $v_0 = \frac{\alpha}{y}$ (Appendix E). The transcendental equation for the Born approximation becomes:

$$tan\left[\frac{\alpha}{y}\sqrt{\frac{y^2}{\sin^2(y]}-1}\right] = \sqrt{\frac{y^2}{\sin^2(y)}-1}\ . \tag{6.6}$$

6.4. Error Analysis

The values of y, both exact and approximate, for different values of α are presented below in Table 6.1. The approximation error is given by

$$\left(\frac{y_{Born}}{y_{exact}}\right)^2 - 1 \tag{6.7}$$

since $E \sim y^2$. These values are consistent with the series solutions for y, obtained by analytical methods. Only the first two terms were kept for y_{Exact} and y_{Born} , while one term was sufficient for % Error.

$$y_{exact} = \alpha - \frac{\alpha^2}{\pi} + \ldots \tag{6.8}$$

$$y_{Born} = \alpha + \frac{\alpha^3}{9} + \ldots \tag{6.9}$$

$$\%Error = \%Error \cong \frac{200\alpha}{\pi}\ \% \quad . \tag{6.10}$$

The graph of % Error plotted against log (α) is presented in Figure 6.1 .

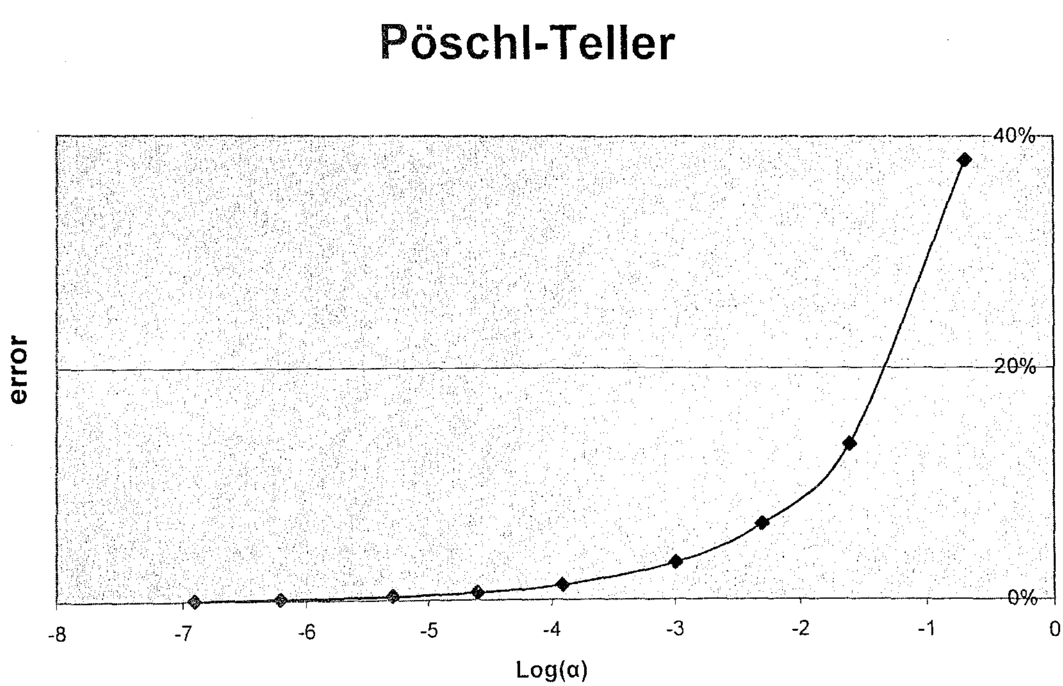

Figure 6.1. % error vs. log (α) for Pöschl-Teller

7. CONCLUSION

In this work we attempted to develop and test a method to estimate the ground state energies of one dimensional potential wells. We first sliced the well into many thin wells, then approximated each by a Dirac delta well. Using Transfer and $\mathbb{S}$-Matrix techniques we solved for the approximate energy levels of this infinite sequence of Dirac delta wells. It was seen that this method is the familiar first Born approximation of scattering, extended to bound states. For calculational simplicity we limited ourselves to potentials satisfying V(x) = V(-x) , but the method may easily be generalized to arbitrary potential functions. The method reduces the Schrödinger differential equation to a transcendental equation involving the Fourier transform of V(x) . After testing the self consistency of the method for a single Dirac delta well, we applied it to three potential problems: double delta well, finite square well and the Pöschl-Teller potentials. The accuracy of the results for narrow and shallow potentials is remarkable. A summary of our results is presented in the equation below and in the table at the end of this section:

$$\tan\sqrt{v^2 - v_0^2} = \frac{\sqrt{v^2 - v_0^2}}{v_0} \tag{7.1}$$

We should point out, however, that there is an essential and fundamental difference between the validity criteria of the first Born approximation applied to scattering or bound states. For scattering, the approximation is valid when $\frac{\sigma}{2} \ll k_0$, a relationship involving both the strength of the potential and the projectile kinetic energy. For the bound states the analogous relation is $\frac{\sigma a}{2} \ll 1$, a statement involving just the parameters of the potential. This corresponds to $V_{min}a^2 < 4eVA^2$ for atomic physics applications, and $V_{min}a^2 < 20MeVf^2$ for nuclear physics applications, which are reasonable values for most problems in these fields. Solid state physics might even be a better field to satisfy the above condition [7] . In this age of fast electronic computation we can not claim that the above method is superior to well established techniques such as the variation method, but we believe it to be original and more analytic. We plan to extend this work to potential functions such as the Morse, Manning-Rose and the

Rosen-Morse, in the near future.

Table 7.1. Summary

	$V(x;a,\sigma)$	v	v_0
Delta	$-\frac{\hbar^2}{2m}\sigma\delta(x-a)$	$\frac{\alpha}{y}$	$\frac{\alpha}{y}$
$P-Delta$ $P=2N+1$	$-\frac{\hbar^2}{2m}\sigma\sum_{n=-N}^{N}\delta(x-na)$	$\frac{\alpha}{y}\frac{\sinh(Py)}{\sinh(y)}$	$\frac{P\alpha}{y}$
Double Delta	$-\frac{\hbar^2}{2m}\sigma\left[\delta\left(x+\frac{a}{2}\right)+\delta\left(x-\frac{a}{2}\right)\right]$	$2\frac{\alpha}{y}\cosh(y)$	$2\frac{\alpha}{y}$
Square Well	$\begin{cases} -\frac{\hbar^2\sigma}{2ma} & \lvert x\rvert < a/2 \\ 0 & \lvert x\rvert > a/2 \end{cases}$	$\frac{\alpha}{y^2}\sinh(y)$	$\frac{\alpha}{y}$
Pöschl-Teller	$-\frac{\pi\hbar^2\sigma}{4ma\cosh^2\left(\frac{\pi x}{a}\right)}$	$\frac{\alpha}{\sin(y)}$	$\frac{\alpha}{y}$

APPENDIX A: EQUIVALENCE TO PATH INTEGRATION

At this point it is proper to correct a possible misconception. Approximating an arbitrary potential well by a sequence of Dirac delta wells and forming an ordered product of their transfer matrices may give the false impression that we only consider the forward motion of the particle, ignoring internal reflection. Counter to naive intuition, this impression is not correct, transferring of coefficients should not be confused with the transfer of particles. To demonstrate our point, let us limit ourselves to the simple scattering problem of two identical delta wells. The overall reflection amplitude consists of an infinite sum of processes : reflection from the first well, transmission through the first well followed by reflection from the second well and transmission through the first well, etc. The transmission amplitude, which is independent of the location of the well, as well as the direction of transmission is given by $t = \frac{1}{1-\frac{i\sigma}{2k_0}}$. The reflection amplitude, on the other hand depends both on the location of the Dirac delta well and the region in which reflection occurs. These amplitudes are given by

$$r^{(L)} = e^{2ik_0x_j} \frac{\frac{i\sigma}{2k_0}}{1 - \frac{i\sigma}{2k_0}} = e^{2ik_0x_j}\, \mathbf{r_0} \quad \texttt{(left to left)} \tag{A.1}$$

$$r^{(R)} = e^{-2ik_0x_j} \frac{\frac{i\sigma}{2k_0}}{1 - \frac{i\sigma}{2k_0}} = e^{-2ik_0x_j}\, \mathbf{r_0} \quad \texttt{(right to right)} \tag{A.2}$$

Forming the infinite series

$$r_T = r_1^{(L)} + tr_2^{(L)}t + tr_2^{(L)}r_1^{(R)}r_2^{(L)}t + \ldots \tag{A.3}$$

and placing the first well at $x = 0$, the second at $x = a$

$$r_T = r_1^{(L)} + t\left[r_2^{(L)} + r_2^{(L)}r_1^{(R)}r_2^{(L)} + \ldots\right]t \tag{A.4}$$

turns into a sum containing a geometric series

$$r_T = r_1^{(L)} + t\left[e^{2ik_0a}\,\mathbf{r_0} + e^{2ik_0a}\,\mathbf{r_0^3} + \ldots\right]t \tag{A.5}$$

which may be summed as

$$r_T = r_0 + \frac{e^{2ik_0a}\,\mathbf{r_0}t^2}{1 - e^{2ik_0a}\,\mathbf{r_0^2}} \tag{A.6}$$

Simplifying and substituting we obtain

$$r_T = \frac{i\sigma}{2k_0}\frac{\left[\left(1+\frac{i\sigma}{2k_0}\right) + e^{2ik_0a}\left(1-\frac{i\sigma}{2k_0}\right)\right]}{\left(1-\frac{i\sigma}{2k_0}\right)^2 + e^{2ik_0a}\frac{\sigma^2}{4k_0^2}}. \tag{A.7}$$

Replacing k_0 by $i\kappa_0$ to study the bound states and defining $\alpha = \frac{\sigma a}{2}$ and $y = \kappa_0 a$ we reach the familiar correct expression.

$$r_T = \frac{\alpha}{y}\frac{\left(1-\frac{\alpha}{y}\right) + \left(1+\frac{\alpha}{y}\right)e^{-2y}}{\left(1-\frac{\alpha}{y}\right)^2 + \frac{\alpha^2}{y^2}e^{-2y}}. \tag{A.8}$$

An alternate and much simpler method would be to form the product

$$\mathbb{M}_{\mathbb{T}} = \mathbb{M}(a)\,\mathbb{M}(0) = \begin{bmatrix} 1+\frac{\alpha}{y} & \frac{\alpha}{y}e^{-2\kappa_0 a} \\ -\frac{\alpha}{y}e^{-2\kappa_0 a} & 1-\frac{\alpha}{y} \end{bmatrix}\begin{bmatrix} 1+\frac{\alpha}{y} & \frac{\alpha}{y} \\ -\frac{\alpha}{y} & 1-\frac{\alpha}{y} \end{bmatrix} \tag{A.9}$$

and to use

$$r_T = [\mathbb{S}_T]_{21} = -\frac{[\mathbb{M}]_{21}}{[\mathbb{M}]_{22}} = \frac{\alpha}{y}\frac{\left(1-\frac{\alpha}{y}\right) + \left(1+\frac{\alpha}{y}\right)e^{-2y}}{\left(1-\frac{\alpha}{y}\right)^2 - \frac{\alpha^2}{y^2}e^{-2y}}. \tag{A.10}$$

Thus we demonstrate that the ordered product of transfer matrices takes into account all possible processes that lead to an overall reflection. When we extend the transfer matrix product method to an infinite sequence of Dirac delta wells, the result is equivalent to the result obtained by a path integral method which takes into account all possible paths within the interaction region.

APPENDIX B: INVARIANCE OF THE ENERGY SPECTRUM UNDER SPACE TRANSLATIONS

Transfer matrices for Dirac delta wells

$$V(x) = -\frac{\hbar^2 \sigma}{2m}\, \delta(x - x_j) \tag{B.1}$$

have the general form:

$$\mathbb{M} = \begin{bmatrix} 1 + \frac{i\sigma_j}{2k_0} & \frac{i\sigma_j}{2k_0} e^{-2ik_0 x_j} \\ -\frac{i\sigma_j}{2k_0} e^{2ik_0 x_j} & 1 - \frac{i\sigma_j}{2k_0} \end{bmatrix} \tag{B.2}$$

or

$$\mathbb{M} = \begin{bmatrix} 1 + \frac{i\sigma_j}{2k_0} & \frac{i\sigma_j}{2k_0} \frac{1}{\lambda_j} \\ -\frac{i\sigma_j}{2k_0} \lambda_j & 1 - \frac{i\sigma_j}{2k_0} \end{bmatrix} , \tag{B.3}$$

where we have defined the only position dependent term $e^{2ik_0 x_j}$ as λ_j. Using a more abstract notation

$$\mathbb{M} = \begin{bmatrix} H_0 & H_{-1} \\ H_1 & H_0 \end{bmatrix} , \tag{B.4}$$

where H_0 , H_1 , H_{-1} denote homogeneous functions of λ with degrees 0, +1 and -1 respectively. Using the multiplication table:

We see that the product of an arbitrary number of transfer matrices will again have the form : $\mathbb{M} = \begin{bmatrix} H_0 & H_{-1} \\ H_1 & H_0 \end{bmatrix}$. Thus $[\mathbb{M}_{\mathbb{T}}]_{22}$, the element that uniquely determines the energy spectrum, belongs to class H_0 and contains only ratios such as $\frac{e^{2ik_0 x_l}}{e^{2ik_0 x_m}}$, which are invariant under the transformation : $x \to x + x_0$. This completes the proof of the invariance of energy spectrum under space translations.

Table B.1. Multiplication Table

	H_0	H_1	H_{-1}
H_0	H_0	H_1	H_{-1}
H_1	H_1	H_2	H_0
H_{-1}	H_{-1}	H_0	H_{-2}

APPENDIX C: BORN APPROXIMATION

$$\left[\frac{\hbar^2 \mathbb{K}^2}{2m} + V(\mathbb{X})\right] |\Psi\rangle = \frac{\hbar^2 k_0^2}{2m} |\Psi\rangle \tag{C.1}$$

$$\left[\mathbb{K}^2 - k_0^2\right] |\Psi\rangle = -\frac{2m\, V(\mathbb{X})}{\hbar^2} |\Psi\rangle \tag{C.2}$$

$$k_0^2 \gg \frac{2m\, |V|_{max}}{\hbar^2} \quad \Rightarrow \quad |\Psi\rangle \approx |k_0\rangle \tag{C.3}$$

$$\left[\mathbb{K}^2 - k_0^2\right] |\Psi\rangle = -\frac{2m\, V(\mathbb{X})}{\hbar^2} |k_0\rangle \tag{C.4}$$

$$|\Psi\rangle \cong |k_0\rangle - \frac{2m}{\hbar^2} \left[\mathbb{K}^2 - k_0^2\right]^{-1} V(\mathbb{X}) |k_0\rangle \cong |k_0\rangle + r\, |-k_0\rangle \tag{C.5}$$

$$-\frac{2m}{\hbar^2} \left[\mathbb{K}^2 - k_0^2\right]^{-1} V(\mathbb{X}) |k_0\rangle \approx r\, |-k_0\rangle \tag{C.6}$$

$$-\frac{2m}{\hbar^2} \int_{-\infty}^{\infty} dk \left[\mathbb{K}^2 - k_0^2\right]^{-1} |k\rangle \langle k |V(\mathbb{X})| k_0\rangle \approx r\, |-k_0\rangle \tag{C.7}$$

$$-\frac{2m}{\hbar^2} \int_{-\infty}^{\infty} dk \frac{\langle k |V(\mathbb{X})| k_0\rangle}{k^2 - k_0^2} |k\rangle \cong r\, |-k_0\rangle \ . \tag{C.8}$$

We must choose the contour such that the pole at $k = -k_0$ is included, while the pole at $k = +k_0$ is excluded. Further the contour must be closed from below since we are

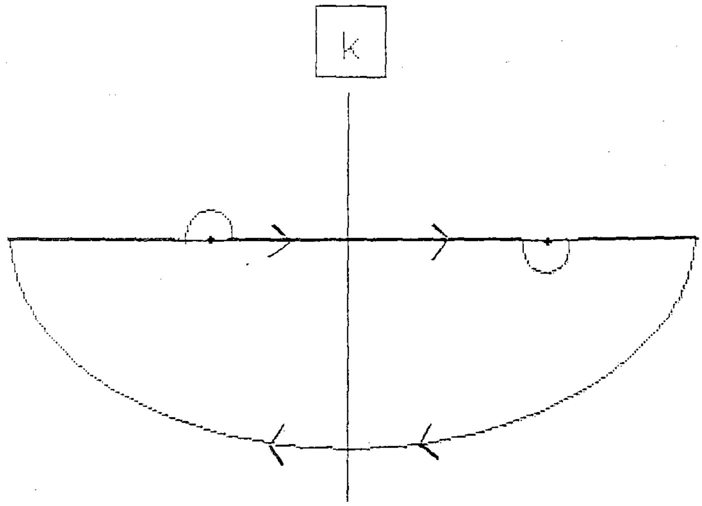

Figure C.1. Integration Contour for Born Approximation

doing our measurement at $x = -\infty$ and $\Psi \sim e^{ikx} \approx e^{ik(-\infty)}$ is regular $\Longleftrightarrow$ $Im\,(k) < 0$

$$\begin{aligned} &-\tfrac{2m}{\hbar^2}\int_{-\infty}^{\infty} dk \tfrac{\langle k|V(\mathbb{X})|k_0\rangle}{(k+k_0)(k-k_0)}\,|k\rangle = \\ &-\tfrac{2m}{\hbar^2}\,(-2\pi i)\,\tfrac{\langle -k_0|V(\mathbb{X})|k_0\rangle}{-2k_0}\,|-k_0\rangle \quad \cong r\,|-k_0\rangle \\ \Rightarrow \quad & r \approx -2\pi i \tfrac{m}{\hbar^2 k_0}\,\langle -k_0\,|V\,(\mathbb{X})|\,k_0\rangle \ . \end{aligned} \tag{C.9}$$

Remembering

$$\langle -k_0\,|V\,(\mathbb{X})|\,k_0\rangle = \frac{1}{\sqrt{2\pi}}\tilde{V}\,(-2k_0) \tag{C.10}$$

we finally obtain

$$r \approx -\frac{\sqrt{2\pi} i\, m}{\hbar^2 k_0}\tilde{V}\,(-2k_0) \ . \tag{C.11}$$

APPENDIX D: v FOR PERIODIC DIRAC DELTA WELLS

We consider the case with P Dirac delta wells

$$P \equiv 2N+1, \quad N = 0,1,2,\ldots \tag{D.1}$$

which can be represented by the potential

$$V(x) = \frac{\hbar^2}{2m}\sigma \sum_{n=-N}^{N} \delta(x-na) \quad . \tag{D.2}$$

We define v as

$$v = -\frac{m}{\hbar^2 \kappa_0}\int_{-\infty}^{\infty} dx\ e^{2\kappa_0 x}\ V(x) \tag{D.3}$$

and v_0 as

$$v_0 = -\frac{m}{\hbar^2 \kappa_0}\int_{-\infty}^{\infty} dx\ V(x) \quad . \tag{D.4}$$

Substituting Equation (D.2) into (D.4)

$$v = \frac{\sigma}{2\kappa_0}\sum_{n=-N}^{N}\int_{-\infty}^{\infty} dx\ e^{2\kappa_0 x}\delta(x-na) \quad . \tag{D.5}$$

Calculating the integral we get

$$\frac{\sigma}{2\kappa_0}\sum_{n=-N}^{N} e^{2\kappa_0 na} \quad . \tag{D.6}$$

Let us define

$$u \equiv e^{2\kappa_0 a} \quad , \tag{D.7}$$

so v can be written as

$$v = \frac{\sigma}{2\kappa_0} \sum_{n=-N}^{N} u^n \ . \tag{D.8}$$

Factoring out $u^{(-N)}$ in the above equation and get

$$v = \frac{\sigma}{2\kappa_0} u^{-N} \left(1 + u + u^2 + \ldots + u^{2N}\right) \tag{D.9}$$

$$\frac{\sigma}{2\kappa_0} \frac{u^{N+1} - u^{-N}}{u - 1} \ . \tag{D.10}$$

$$v = \frac{\sigma}{2\kappa_0} \frac{u^{N+\frac{1}{2}} - u^{-\left(N+\frac{1}{2}\right)}}{u^{\frac{1}{2}} - u^{-\frac{1}{2}}} \ . \tag{D.11}$$

Substituting $e^{2\kappa_0 a} = u$

$$\frac{\sigma}{2\kappa_0} \frac{e^{P\kappa_0 a} - e^{-P\kappa_0 a}}{e^{\kappa_0 a} - e^{-\kappa_0 a}} \tag{D.12}$$

$$\frac{\sigma}{2\kappa_0} \frac{\sinh\left(P\kappa_0 a\right)}{\sinh\left(\kappa_0 a\right)} \ . \tag{D.13}$$

Using the limit $v_0 = \frac{1}{\kappa_0} \lim_{\kappa_0 \to 0} \left(\kappa_0 v\right)$ we obtain the final result

$$v_0 = \frac{\sigma P}{2\kappa_0} \ . \tag{D.14}$$

APPENDIX E: v FOR PÖSCHL-TELLER POTENTIAL

We defined v as

$$v = -\frac{2m}{\hbar^2 \kappa_0} \int_0^\infty dx \cosh\left(2\kappa_0 x\right) v\left(x\right) \tag{E.1}$$

where $V\left(x\right)$ is the so-called Pöschl-Teller potential

$$V\left(x\right) = -\frac{\pi \hbar^2 \sigma}{4ma} \frac{1}{\cosh^2\left(\frac{\pi x}{a}\right)} \quad . \tag{E.2}$$

Therefore

$$v 0 \frac{\pi \sigma}{2\kappa_0 a} \int_0^\infty dx \, \frac{\cosh\left(2\kappa_0 x\right)}{\cosh^2\left(\frac{\pi x}{a}\right)} \quad . \tag{E.3}$$

$$v = \frac{\sigma}{2\kappa_0 a} \beta \left(1 + \frac{\kappa_0 a}{\pi} \,,\, 1 - \frac{\kappa_0 a}{\pi}\right) \qquad \left(\kappa_0 < \frac{\pi}{a}\right) \tag{E.4}$$

$$\begin{aligned} v &= \tfrac{\alpha}{y} \Gamma\left(1 + \tfrac{y}{\pi}\right) \Gamma\left(1 - \tfrac{y}{\pi}\right) \qquad (y < \pi) \\ &= \tfrac{\alpha}{y} \Gamma\left(1 + \tfrac{y}{\pi}\right) \Gamma\left(1 + \tfrac{y}{\pi}\right) \\ &= \tfrac{\alpha}{\sin(y)} \quad . \end{aligned} \tag{E.5}$$

Formulas 3.512.1, 8.331, 8.334.3 of Reference [8] . While

$$v_0 = \frac{1}{y} \lim_{y \to 0} \left(yv\right) = \frac{\alpha}{y} \quad . \tag{E.6}$$

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