Progressively accurate WKB approximations through factorization and successive boost transformations

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Abstract

This paper develops a procedure for obtaining progressively improving approximate solutions of the WKB (semiclassical) model of the stationary Schroedinger equation through factorization and successive boost transformations of the resultant equivalent matrix equation. Each order of approximation provides an amplitude-modulated "plane" wave function specified by a *renormalized momentum*. A simple binomial expansion of the renormalized momentum allows exact evaluation of the phase accumulation integral for studying basic features of the dynamics in arbitrary potentials. For a linear potential, the probability density profile reveals the expected confinement of the particle within the allowed energy region.

Keywords: factorization; matrix form; accuracy levels; boost transformation; renormalized momentum; confinement

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1 Introduction

In the WKB (semiclassical) model of approximate solutions, the stationary Schroedinger equation for a particle of mass m and total energy E in a field potential $V(x)$ is expressed in the form

$$(\hbar^2 \frac{d^2}{dx^2} + p^2)\psi = 0 \tag{1a}$$

where $p(x)$ is the linear momentum obtained as

$$p(x) = \sqrt{2m(E - V(x))} \tag{1b}$$

The model in equations $(1a)$-$(1b)$ is useful in describing potential barrier penetration and quantum tunneling phenomena.

Assuming that the potential $V(x)$ varies slowly in space, approximate solutions of equation $(1a)$ can be obtained by imposing the WKB approximation condition [1-3]

$$\frac{\hbar}{p^2}\frac{dp}{dx} \;=\; \frac{1}{k^2}\frac{dk}{dx} \ll 1 \quad ; \quad p = \hbar k \tag{1c}$$

where k is the wave number. For later reference, we introduce the "WKB approximation parameter " w defined by

$$w = \frac{\hbar}{p^2}\frac{dp}{dx} \;=\; \frac{1}{k^2}\frac{dk}{dx} \quad \Rightarrow \quad w << 1 \tag{1d}$$

Starting with ansatz of the form

$$\psi(x) = e^{i\phi(x)} \tag{1e}$$

and imposing the approximation condition $(1c)$ provides the leading order in the allowed energy region $E > V(x)$, expressed in the asymptotic form [1-14]

$$\psi_{wkb}(x) = \frac{A}{\sqrt{p(x)}} e^{-\frac{i}{\hbar}\int_{x_0}^{x} p(x')\ dx'} + \frac{B}{\sqrt{p(x)}} e^{\frac{i}{\hbar}\int_{x_0}^{x} p(x')\ dx'} \quad ; \quad E > V(x) \tag{1f}$$

which in the asymptotic limit takes the form

$$\psi_{wkb}(x) = \frac{C}{\sqrt{p(x)}} \cos(\frac{1}{\hbar}\int_{x_0}^{x} p(x')\ dx' \mp \frac{\pi}{4}) \quad ; \quad E > V(x) \tag{1g}$$

The WKB leading order probability density $\rho_{wkb}(x)$ is obtained as

$$\rho_{wkb}(x) = |\overline{\psi}_{wkb}(x)|^2 \quad ; \quad \overline{\psi}_{wkb}(x) = \frac{\psi_{wkb}(x)}{C} \tag{1h}$$

Taking the linear potential $V(x) = \kappa x$ as a useful example for comparison with results obtained in the present paper, we plot $\rho_{wkb}(x)$ in Fig. 1 using $\psi_{wkb}(x)$ from equation $(1g)$. We observe that the probability density profile in the allowed energy region $E > \kappa x$ undergoes a discontinuity near the energy turning point $E = \kappa x$, without displaying any features of the confining property of the linear potential.

$$\rho_{wkb}(x) \quad \text{for} \quad V(x) = \kappa x \quad , \quad p(x) = \sqrt{b - ax} \quad , \quad b = 2mE \ , \ a = 2m\kappa \quad ; \quad \vartheta = \frac{\pi}{4} \qquad (1i)$$

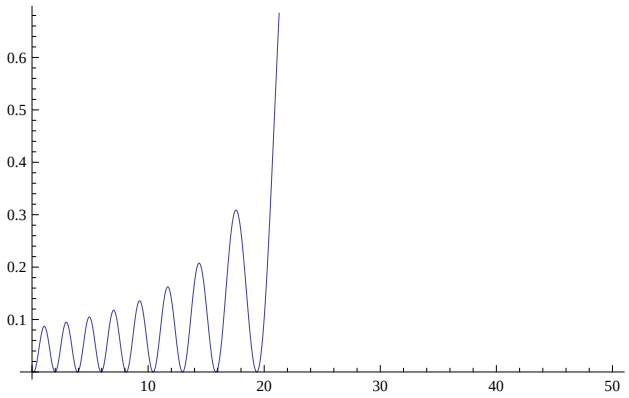

Figure 1: WKB probability density $\rho_{wkb}(x)$ $(1h)$ using $\psi_{wkb}(x)$ $(1g)$ for linear potential $V(x) = \kappa x$ with $b = 12$, $a = 0.5$, over the range $x = 0 \rightarrow 50$

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Even though the WKB approximation was based on a very slowly varying potential $V(x)$ in non-relativistic quantum mechanics, the leading order form in equation $(1f)$ and its improvements through some appropriate forms of series expansions has also been widely applied to investigations of systems of varying forms of potentials in relativistic physics, notably cosmology, Dirac equation and quarkonium physics [7-14].

A very serious problem with the WKB method is that it is too difficult to improve the accuracy beyond the leading order form in equation $(1f)$. The standard method of expanding the arbitrary phase $\phi(x)$ in equation $(1e)$ in powers of $\hbar$ through perturbation or other suitable series expansion methods [1-14] always run into difficulties after only a few orders as the calculation gets more tedious at every step and the series expansions may also be divergent beyond some terms. In addition, the validity of the approximation condition $(1c)$ may also be questionable since the WKB approximation parameter $w(x) = \frac{\hbar}{p^2}\frac{dp}{dx}$ may not be very small for some potentials $V(x)$.

In the present paper, we develop a new solution procedure which automatically overcomes the major challenges of the WKB or power series expansion methods stated above. We factorize and express the stationary Schroedinger equation $(1a)$ in an appropriate matrix form. A general solution up to a desired n^{th}-order approximation is obtained by first transforming the matrix equation to a suitable boost frame through n successive boost transformations alternately along the x-axis and y-axis. Each boost transformation provides an approximate diagonalized Hamiltonian matrix specified by a *renormalized momentum* and a smaller approximation parameter. The ever reducing magnitude of the approximation parameter means that each boost operation improves the accuracy of the approximate solution. An important outcome of the boost operations is that the resulting renormalized momentum has a simple binomial expansion in powers of the corresponding approximation parameter, which facilitates exact evaluation of the phase accumulation integral for various forms of the potential $V(x)$. The resulting wave function and corresponding probability density display expected behavior for arbitrary entry-boundary angles within the allowed energy region, with discontinuities occurring only near well defined turning points.

2 Factorization

The form of the second-order differential operator $(\hbar^2 \frac{d^2}{dx^2} + p^2)$ in equation $(1a)$ shows that it is expressible as a difference of two squares after introducing the imaginary number $i = \sqrt{-1}$ according to $a^2 + b^2 = a^2 - (ib)^2$, which is easily factorized, depending on the forms of a and b. Applying this in equation $(1a)$ and taking account of the x-dependence of $p(x)$ provides two alternative factorized forms

$$(-i\hbar\frac{d}{dx} + p)(i\hbar\frac{d}{dx} + p)\psi = -i\hbar\frac{dp}{dx}\psi \tag{2a}$$

$$(i\hbar\frac{d}{dx} + p)(-i\hbar\frac{d}{dx} + p)\psi = i\hbar\frac{dp}{dx}\psi \tag{2b}$$

according to the ordering of the differential operators.

Introducing complex *wave amplitudes* ϕ and ϕ^* defined by

$$\sqrt{p}\ \phi = (i\hbar\frac{d}{dx} + p)\psi \quad ; \quad \sqrt{p}\ \phi^* = (-i\hbar\frac{d}{dx} + p)\psi \quad \Rightarrow \quad \psi = \frac{1}{2\sqrt{p}}(\phi + \phi^*) \tag{3a}$$

we express equations $(2a)$-$(2b)$ in the simpler first-order forms

$$i\hbar\frac{d\phi}{dx} = p\ \phi + i\frac{\hbar}{2p}\frac{dp}{dx}\ \phi^* \quad ; \quad i\hbar\frac{d\phi^*}{dx} = -p\ \phi^* + i\frac{\hbar}{2p}\frac{dp}{dx}\ \phi \tag{3b}$$

These are coupled equations for the wave amplitudes ϕ and ϕ^*. We identify a *factorization coupling parameter* $f(x)$ defined by

$$f(x) = \frac{\hbar}{2p}\frac{dp}{dx} \tag{3c}$$

which we substitute into equation $(3b)$ to obtain the final form

$$i\hbar\frac{d\phi}{dx} = p\ \phi + if\ \phi^* \tag{3d}$$

$$i\hbar\frac{d\phi^*}{dx} = -p\ \phi^* + if\ \phi \tag{3e}$$

An important point to note is that for real ψ, the wave amplitudes ϕ and ϕ^* as defined in equation $(3a)$ are complex conjugates, while for complex ψ, the wave amplitudes ϕ and ϕ^* would not be related by simple complex conjugation. However, equations $(3a)$-$(3b)$ apply for real or complex ψ, since they follow from the operator ordering in the factorization and definitions given in equations $(2a)$-$(2b)$ and $(3a)$, respectively. We may then adopt general notation

$$\phi \to \phi_- \quad ; \quad \phi^* \to \phi_+ \quad ; \quad \psi = \frac{1}{2\sqrt{p}}(\phi_- + \phi_+) \tag{3f}$$

defined according to equation $(3a)$, applying to real ψ $(\phi_+ = \phi_-^*)$ or complex ψ $(\phi_+ \neq \phi_-^*)$.

2.1 The matrix form

Introducing a two-component column matrix χ defined by

$$\chi = \begin{pmatrix} \phi \\ \phi^* \end{pmatrix} \tag{4a}$$

equations $(3d)$-$(3e)$ are expressed in the matrix form

$$i\hbar\frac{d\chi}{dx} = H\chi \tag{4b}$$

where H is the corresponding 2×2 Hamiltonian matrix obtained as

$$H = \begin{pmatrix} p & if \\ if & -p \end{pmatrix} \tag{4c}$$

We use the Pauli spin matrices σ_z and σ_x defined by

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad ; \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{4d}$$

to express the Hamiltonian matrix in the form

$$H = p\sigma_z + if\sigma_x \tag{4e}$$

We complete the specification of Pauli matrices by introducing the identity I and σ_y defined as

$$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad ; \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \tag{4f}$$

In general, exact analytical solution of the matrix equation $(4b)$ cannot be obtained through direct integration due to the x-dependence of the coefficients $p(x)$ and $f(x)$ of the Hamiltonian H in equation $(4e)$. In an arbitrarily varying potential $V(x)$, the Hamiltonian $H(x)$ at point x may not commute with $H(x')$ at a different point x', which means that space coordinate ordering can affect the results. Direct integration may apply only as an approximation in the case of very slowly varying potential where $[H(x)\ ,\ H(x')] \approx 0$.

3 Accuracy levels, dynamical frames and transformations

An approximation procedure is considered good if it is consistent and can achieve high accuracy. Accuracy is a measure of the validity of the approximation conditions which determine the effectiveness of the approximation procedure. In standard practice, approximation conditions are specified by approximation parameters which are either small enough to be neglected or can be used as expansion parameters in power series expansions. Neglecting an approximation parameter or terminating a series expansion in powers of the approximation parameter at some order determines the level of accuracy achievable. In some cases, series expansions may either be divergent or get too complicated to be evaluated exactly beyond the first few orders. Divergence completely destroys accuracy and validity of approximation procedure, while termination at low orders of expansion limits the level of accuracy. We provide an alternative procedure for improving accuracy of approximation through successive transformations in the present paper.

On the general understanding that accuracy is described as low , fair or high, we adopt an interpretation that accuracy is classified in terms of levels, from low to high accuracy. We consider that an accuracy level is defined on a dynamical frame and that improving from one accuracy level to a higher accuracy level is equivalent to an advancement from one dynamical frame of lower accuracy level to another dynamical frame of higher accuracy level. The advancement from one accuracy

level to a higher accuracy level is then interpreted as a transformation from a dynamical frame of lower accuracy to another dynamical frame of higher accuracy through application of an appropriate transformation operator T. Each operation has the effect of reducing the size of the approximation parameter, thereby improving the accuracy. We specify the original dynamical frame (where the equation of dynamics $(1a)$ applies) as the *zeroth* or leading-order dynamical frame. The approximation parameter defined in the original frame is called *zeroth-order approximation parameter*, ξ_0, which normally satisfies $\xi_0 < 1$ and corresponds to lowest level accuracy. In the dynamics governed by the stationary Schroedinger equation $(1a)$, we shall determine ξ_0 to be equal to half the usual WKB approximation parameter.

Starting from the original dynamical frame of *zero-order* (lowest level) accuracy, we apply $n \geq 1$ successive transformation operations to reach the n^{th} dynamical frame of n^{th}-order (higher) accuracy. The zeroth-order transformation operator $T = T_0$ is an *identity operator* which leaves the original frame invariant. The *first-order* transformation operator composed as $T = T_1 T_0$ transforms the original dynamical frame to the first-order dynamical frame characterized by the first-order approximation parameter ξ_1 obtained in terms of a first-order derivative of the zeroth-order approximation parameter ξ_0 and therefore $\xi_1 < \xi_0$ as established in the next section. The n^{th}-order transformation operator composed as $T = T_n T_{n-1} .... T_1 T_0$ transforms the original dynamical frame to the n^{th}-order dynamical frame characterized by the n^{th}-order approximation parameter ξ_n, which is obtained in terms of the n^{th}-order derivative of ξ_0, such that $\xi_n \ll \xi_0$. Accuracy then increases progressively under successive transformations from the zeroth-order to the n^{th}-order dynamical frame. Each transformation operator T_n is specified by an arbitrary transformation parameter θ_n, which is eliminated at the end of the operation with T_n to determine the form of ξ_n before applying the next operator T_{n+1}.

3.1 The transformation law

We develop the transformation law by considering that the transformation from one dynamical frame to another of higher accuracy level is taken one step at a time. In this respect, we consider the general case of a transformation from the n^{th}-order dynamical frame characterized by wave amplitude matrix χ_n, Hamiltonian H_n, approximation parameter ξ_n and transformation operator T_n specified by arbitrary transformation parameter θ_n, to the $(n+1)^{th}$-order dynamical frame. The equation of dynamics in the n^{th}-order dynamical frame takes the form

$$i\hbar \frac{d\chi_n}{dx} = H_n \chi_n \quad , \quad n = 0, 1, 2, 3, ..., \tag{5a}$$

Transformation to the $(n+1)^{th}$-order dynamical frame characterized by wave amplitude χ_{n+1} and transformation operator T_{n+1} is defined by

$$\chi_{n+1} = T_{n+1} \chi_n \qquad \Rightarrow \qquad \chi_n = T_{n+1}^{-1} \chi_{n+1} \tag{5b}$$

In general, a transformation operator T and its inverse T^{-1} satisfy the condition

$$T T^{-1} \; = \; T^{-1} T = I \tag{5c}$$

where I is the identity matrix.

We substitute $\chi_n = T_{n+1}^{-1} \chi_{n+1}$ from equation $(5b)$ into equation $(5a)$, multiply the result by T_{n+1} from the left and then apply the condition $(5c)$ to obtain the equation of dynamics in the $(n+1)^{th}$-order dynamical frame in the form

$$i\hbar \frac{d\chi_{n+1}}{dx} = H_{n+1} \chi_{n+1} \quad , \quad n = 0, 1, 2, 3, ..., \tag{5d}$$

where the Hamiltonian H_{n+1} is obtained as a transformation of H_n according to

$$H_{n+1} = T_{n+1} H_n T_{n+1}^{-1} - i\hbar T_{n+1} \frac{dT_{n+1}^{-1}}{dx} \tag{5e}$$

3.2 The boost frames

According to equation $(4e)$, the original Hamiltonian H is non-Hermitian. We therefore consider that the appropriate transformation to apply is a *boost* along an axis *normal* to the plane of the Hamiltonian. In the general terminology adopted in the present work, the zeroth-order dynamical frame Hamiltonian $H_0 = H$ given in equation $(4e)$ is expressed as

$$H_0 = q_0\sigma_z + i\xi_0\sigma_x \tag{6a}$$

where we call $q_0(x)$ and $\xi_0(x)$ the zeroth-order *renormalized momentum* and *dynamical approximation parameter*, respectively defined by comparing equations $(4e)$ and $(6a)$ in the form

$$q_0 = p \quad ; \quad \xi_0 \;=\; f = \frac{\hbar}{2p}\frac{dp}{dx} \tag{6b}$$

The fact that $H_0 = H$ is defined in the zx-plane means that the original (zeroth-order) dynamical frame of the stationary Schroedinger equation is the zx-plane. The first-order boost operator $T_1(x)$ is therefore defined along the y-axis specified by an arbitrary transformation parameter $\theta_1(x)$ according to the definition

$$T_1(x) = e^{\frac{1}{2}\theta_1(x)\sigma_y} = \begin{pmatrix} \cosh\frac{1}{2}\theta_1 & -i\sinh\frac{1}{2}\theta_1 \\ i\sinh\frac{1}{2}\theta_1 & \cosh\frac{1}{2}\theta_1 \end{pmatrix} \tag{6c}$$

which on substituting into equation $(5e)$ for $n = 0$, $H_0 = H$ and then eliminating the arbitrary $\theta_1(x)$ as explained below provides the first-order dynamical frame Hamiltonian H_1 in the form

$$H_1 = q_1\sigma_z - i\xi_1\sigma_y \tag{6d}$$

where $q_1(x)$ and $\xi_1(x)$ are the first-order renormalized momentum and dynamical approximation parameter, respectively. We observe that H_1 is defined in the zy-plane, meaning that the first-order dynamical frame is the zy-plane. The transformation from the first-order dynamical frame is therefore a boost along the x-axis.

In general, the accuracy level dynamical frames alternate between zx and zy planes so that the corresponding boost transformations along axes normal to the dynamical planes are effected by boost transformations defined alternately along y-axis or x-axis as appropriate. For the general transformation from the n^{th}-order frame to the $(n+1)^{th}$-order frame specified above, we define T_{n+1} and its inverse T_{n+1}^{-1} in relation to the plane of H_n according to

$$H_n = q_n\sigma_z - i\xi_n\sigma_x \qquad \Rightarrow \qquad T_{n+1}(x) = e^{\frac{1}{2}\theta_{n+1}(x)\sigma_y} = \begin{pmatrix} c_{n+1} & -is_{n+1} \\ is_{n+1} & c_{n+1} \end{pmatrix}$$

$$T_{n+1}^{-1}(x) = e^{-\frac{1}{2}\theta_{n+1}(x)\sigma_y} = \begin{pmatrix} c_{n+1} & is_{n+1} \\ -is_{n+1} & c_{n+1} \end{pmatrix} \tag{7a}$$

which we substitute into the transformation law in equation $(5e)$ to obtain

$$H_{n+1} = q_n\{(\cosh\theta_{n+1} + \bar{\xi}_n\sinh\theta_{n+1})\sigma_z - i(\sinh\theta_{n+1} + \bar{\xi}_n\cosh\theta_{n+1})\sigma_x\} + i\frac{\hbar}{2}\frac{d\theta_{n+1}}{dx}\,\sigma_y \tag{7b}$$

while the form

$$H_n = q_n\sigma_z - i\xi_n\sigma_y \quad \Rightarrow \quad T_{n+1}(x) = e^{\frac{1}{2}\theta_{n+1}(x)\sigma_x} = \begin{pmatrix} c_{n+1} & s_{n+1} \\ s_{n+1} & c_{n+1} \end{pmatrix}$$

$$T^{-1}_{n+1}(x) = e^{-\frac{1}{2}\theta_{n+1}(x)\sigma_x} = \begin{pmatrix} c_{n+1} & -s_{n+1} \\ -s_{n+1} & c_{n+1} \end{pmatrix} \tag{7c}$$

substituted into equation $(5e)$ gives

$$H_{n+1} = q_n\{(\cosh\theta_{n+1} + \overline{\xi}_n \sinh\theta_{n+1})\sigma_z - i(\sinh\theta_{n+1} + \overline{\xi}_n\cosh\theta_{n+1})\sigma_y\} + i\frac{\hbar}{2}\frac{d\theta_{n+1}}{dx}\,\sigma_x \tag{7d}$$

where we have introduced short notation for approximation parameter and the hyperbolic functions in the form

$$\overline{\xi}_n = \frac{\xi_n}{q_n} \quad ; \quad c_{n+1} = \cosh\frac{1}{2}\theta_{n+1}(x) \quad ; \quad s_{n+1} = \sinh\frac{1}{2}\theta_{n+1}(x) \tag{7e}$$

We have used standard hyperbolic function identities

$$\cosh^2(.) + \sinh^2(.) = \cosh 2(.) \quad ; \quad 2\sinh(.)\cosh(.) = \sinh 2(.) \tag{7f}$$

to obtain the final form in equations $(7b)$ and $(7d)$.

3.2.1 Eliminating $\theta_{n+1}(x)$: renormalized momentum

The only externally introduced arbitrary parameter in the Hamiltonian H_{n+1} in equations $(7b)$ and $(7d)$ is the boost transformation parameter $\theta_{n+1}(x)$, which must be eliminated to obtain a physically meaningful boost frame Hamiltonian. Since we shall diagonalize H_{n+1} in the end to obtain the desired approximate solution of equation $(5d)$ in the $(n+1)^{th}$-order dynamical frame, we start by eliminating the σ_x-component in equation $(7b)$ or the σ_y-component in equation $(7d)$ by setting the coefficient to zero according to

$$\sinh\theta_{n+1} + \overline{\xi}_n\cosh\theta_{n+1} = 0 \tag{8a}$$

which easily fixes the boost parameter θ_{n+1} in terms of the physical parameters in the form

$$\tanh\theta_{n+1}(x) = -\overline{\xi}_n(x) \tag{8b}$$

Squaring equation $(8b)$ and using $\cosh^2(.) - \sinh^2(.) = 1$ gives

$$\cosh\theta_{n+1}(x) = \frac{1}{\sqrt{1-\overline{\xi}^2_n(x)}} \quad ; \quad \sinh\theta_{n+1}(x) = -\frac{\overline{\xi}_n(x)}{\sqrt{1-\overline{\xi}^2_n(x)}} \tag{8c}$$

where the negative sign in the definition of $\tanh\theta_{n+1}(x)$ has been taken into account in the derivation of $\cosh\theta_{n+1}(x)$ and $\sinh\theta_{n+1}(x)$. We then obtain

$$\cosh\theta_{n+1}(x) + \overline{\xi}_n(x)\sinh\theta_{n+1}(x) = \sqrt{1-\overline{\xi}^2_n(x)} \tag{8d}$$

Differentiating equation $(8b)$ with respect to x using

$$\frac{d}{dx}\tanh\theta_{n+1} = \frac{d\theta_{n+1}}{dx}\frac{d}{d\theta_{n+1}}\tanh\theta_{n+1} = \frac{d\theta_{n+1}}{dx}(1-\tanh^2\theta_{n+1}) \tag{8e}$$

gives the final result

$$\frac{\hbar}{2}\frac{d\theta_{n+1}}{dx} = -\frac{\hbar}{2(1-\overline{\xi}_n^2(x))}\frac{d\,\overline{\xi}_n(x)}{dx} \tag{8f}$$

Noticing that the r.h.s. of equation $(8f)$ involves first-order derivative of the n-order boost approximation parameter $\overline{\xi}_n = \frac{\xi_n}{q_n}$, we introduce the $(n+1)^{th}$ boost approximation parameter $\xi_{n+1}(x)$ defined by

$$\frac{\hbar}{2}\frac{d\theta_{n+1}}{dx} = -\xi_{n+1}(x) \quad \Rightarrow \quad \xi_{n+1}(x) = \frac{\hbar}{2(1-\overline{\xi}_n^2(x))}\frac{d\,\overline{\xi}_n(x)}{dx} \quad , \quad n = 0, 1, 2, 3, ..., \tag{8g}$$

Substituting equations $(8a)$, $(8d)$ and $(8g)$ into equations $(7b)$ and $(7d)$ (noting that the coefficients are the same), we obtain the boost frame Hamiltonian in the alternate forms

$$H_n = q_n\sigma_z - i\xi_n\sigma_x \quad \Rightarrow \quad H_{n+1} = q_{n+1}\sigma_z - i\xi_{n+1}\sigma_y \tag{9a}$$

$$H_n = q_n\sigma_z - i\xi_n\sigma_y \quad \Rightarrow \quad H_{n+1} = q_{n+1}\sigma_z - i\xi_{n+1}\sigma_x \tag{9b}$$

where we have introduced the $(n+1)^{th}$-order *renormalized momentum* $q_{n+1}(x)$ obtained as

$$q_{n+1}(x) = q_n(x)\sqrt{1-\overline{\xi}_n^2(x)} \quad , \quad n = 0, 1, 2, 3, ..., \tag{9c}$$

Setting $n = 0, 2, 3, ...$, in equations $(9a)$-$(9c)$ provides the zeroth, even and odd order dynamical frame Hamiltonians according to

$$H_0 = q_0\sigma_z + i\xi_0\sigma_x \quad ; \quad q_0 = p \quad ; \quad \xi_0 = \frac{\hbar}{2p}\frac{dp}{dx} \quad ; \quad \overline{\xi}_0 = \frac{\xi_0}{q_0} = \frac{1}{2}w \tag{9d}$$

where $w(x)$ is the WKB approximation parameter defined in equation $(1d)$.

$$H_{2n} = q_{2n}\sigma_z - i\xi_{2n}\sigma_x \quad ; \quad q_{2n} = q_{2n-1}\sqrt{1-\overline{\xi}_{2n-1}^2} \quad ; \quad \xi_{2n} = \frac{\hbar}{2(1-\overline{\xi}_{2n-1}^2)}\frac{d\,\overline{\xi}_{2n-1}}{dx}$$

$$\overline{\xi}_{2n-1} = \frac{\xi_{2n-1}}{q_{2n-1}} \quad , \quad n \geq 1 \tag{9e}$$

$$H_{2n+1} = q_{2n+1}\sigma_z - i\xi_{2n+1}\sigma_y \quad ; \quad q_{2n+1} = q_{2n}\sqrt{1-\overline{\xi}_{2n}^2} \quad ; \quad \xi_{2n+1} = \frac{\hbar}{2(1-\overline{\xi}_{2n}^2)}\frac{d\,\overline{\xi}_{2n}}{dx}$$

$$\overline{\xi}_{2n} = \frac{\xi_{2n}}{q_{2n}} \quad , \quad n \geq 0 \tag{9f}$$

3.3 Diagonalization and approximate solutions

We recall that the purpose of the transformations of the original equation $(4b)$ and its Hamiltonian $(4e)$ is to find a dynamical frame in which the resultant Hamiltonian is either space-independent for an exact analytical solution or has a negligible approximation parameter for a high accuracy approximation. Since the renormalized momentum $q_n(x)$ and the dynamical approximation parameter $\xi_n(x)$ which specify the Hamiltonian H_n in the n^{th}-order dynamical frame for $n = 0, 1, 2, 3, ...$, are space-dependent, the resultant equation of dynamics $(5a)$ (note that $(5d)$ takes the same form as $(5a)$ for $n \to n+1$) can only be solved under good approximation conditions in which we consider

the n^{th}-order dynamical approximation parameter $\xi_n(x)$ to be negligible. Under such conditions, the Hamiltonian H_n is diagonalized, leading to a simple solution through direct integration.

The main task is to establish that the n^{th}-order approximation parameter $\xi_n(x)$ is small enough to be neglected at the $n \geq 0$ accuracy level. To do this, we consider that $\xi_n(x)$ is defined in terms of progressively increasing orders of differentiation of the zeroth-order approximation parameter $\xi_0(x)$ according to

$$n = 0 \ : \quad \xi_0 = \frac{\hbar}{2p}\frac{dp}{dx} \quad ; \quad q_0 = p \quad ; \quad \overline{\xi}_0 = \frac{\xi_0}{q_0} = \frac{1}{2}w$$

$$n \geq 1 \ : \quad \xi_n = \frac{\hbar}{2(1-\overline{\xi}_{n-1}^2)}\frac{d\,\overline{\xi}_{n-1}}{dx} \quad ; \quad \overline{\xi}_{n-1} = \frac{\xi_{n-1}}{q_{n-1}} \tag{10a}$$

where $w(x)$ is the WKB approximation parameter. We now consider the cases $n = 1, 2$ to realize the physical implications.

$$n = 1 \ : \quad \xi_1 = \frac{\hbar}{2(1-\overline{\xi}_0^2)}\frac{d\,\overline{\xi}_0}{dx} = \frac{\hbar}{4(1-\frac{1}{4}w^2)}\frac{dw}{dx} \tag{10b}$$

$$n = 2 \ : \quad \xi_2 = \frac{\hbar}{2(1-\overline{\xi}_1^2)}\frac{d\,\overline{\xi}_1}{dx} \quad ; \quad \overline{\xi}_1 = \frac{\xi_1}{q_1} \quad ; \quad \frac{d\,\overline{\xi}_1}{dx} = \frac{d}{dx}(\frac{\xi_1}{q_1}) = \frac{1}{q_1}(\frac{d\xi_1}{dx} - \overline{\xi}_1\frac{dq_1}{dx}) \tag{10c}$$

We use equation $(10b)$ to obtain

$$\frac{d\xi_1}{dx} = \frac{d}{dx}\frac{\hbar}{4(1-\frac{1}{4}w^2)}\frac{dw}{dx} = \frac{\hbar}{4}\{\frac{w}{2(1-\frac{1}{4}w^2)^2}(\frac{dw}{dx})^2 + \frac{1}{(1-\frac{1}{4}w^2)}\frac{d^2w}{dx^2}\} \tag{10d}$$

In general, the dynamical approximation parameters are proportional to the derivatives of the WKB parameter according to the degree

$$\xi_1 \sim \frac{dw}{dx} \quad ; \quad \xi_2 \sim \{(\frac{dw}{dx})^2 \quad , \quad \frac{d^2w}{dx^2}\} \tag{10e}$$

$$n \geq 2 \ : \quad \xi_n \sim \{(\frac{dw}{dx})^n \quad , \quad \frac{d^nw}{dx^n}\} \tag{10f}$$

It is clear that under the WKB approximation condition ($w \ll 1$) in equations $(1c)$-$(1d)$, the dynamical approximation parameters $\xi_n(x)$ become progressively smaller with increasing $n \geq 0$. This means that the accuracy level increases with the number $n \geq 0$ of successive transformations from the zeroth-order to the n^{th}-order ($n \geq 1$) dynamical frame. The highest accuracy level is achieved in the dynamical frame where the approximation parameter $\xi(x)$ takes the smallest possible value and can be safely neglected. Hence, for n^{th}-level accuracy (equivalent to approximation to the n^{th}-order), we set $\xi_n(x)$ (general $n = 0$, even , odd) equal to zero in any of the forms in equations in $(9a)$-$(9e)$, leading to diagonalization of the general n^{th}-order dynamical Hamiltonian according to

$$\xi_0(x) = 0 \quad \Rightarrow \quad H_0 = q_0\sigma_z \quad , \quad q_0(x) = p(x) \quad ; \quad \overline{\xi}_0(x) = \frac{1}{2}w(x) \tag{11a}$$

$$\xi_n(x) = 0 \quad \Rightarrow \quad H_n = q_n\sigma_z \quad , \quad q_n(x) = q_{n-1}(x)\sqrt{1-\overline{\xi}_{n-1}^2(x)} \quad , \quad n = 1, 2, 3, ..., \tag{11b}$$

Substituting the diagonalized Hamiltonian from equations $(11a)$-$(11b)$ into equation $(5a)$, we easily obtain the approximate solution satisfying the accuracy conditions $(11a)$-$(11b)$ in the n^{th}-order dynamical frame in the form

$$\chi_n(x) = U_n(x)\chi_n(0) \quad , \quad n = 0, 1, 2, 3, ..., \tag{11c}$$

with the space evolution operator $U_n(x)$ obtained through direct integration in the final form

$$U_n(x) = e^{-i\delta_n(x)\sigma_z} \quad , \quad n = 0, 1, 2, 3, ..., \tag{11d}$$

where the phase accumulation integral $\delta_n(x)$ has been obtained as

$$\delta_n(x) = \frac{1}{\hbar}\int_{x_0}^{x} q_n(x')dx' \quad , \quad n = 0, 1, 2, 3, ..., \tag{11e}$$

Noting that $\chi_n(x)$ in the n^{th}-order dynamical frame is obtained from $\chi(x)$ as defined in equation $(4a)$ in the original frame through a succession of boost transformations according to

$$\chi_n(x) = T_n(x)\chi_{n-1}(x) = T_n(x)T_{n-1}(x)T_{n-2}(x).....T_3(x)T_2(x)T_1(x)T_0(x)\chi(x) \tag{12a}$$

where

$$T_0(x) = I \quad \Rightarrow \quad \chi_0(x) = T_0(x)\chi(x) = \chi(x) \tag{12b}$$

we apply the inverse operations in succession from the left of equation $(12a)$, starting with $T_n^{-1}(x)$ as appropriate, to obtain the original wave amplitude in the form $(T_0^{-1}x = I)$

$$\chi(x) = T_1^{-1}(x)T_2^{-1}(x)T_3^{-1}(x).....T_{n-2}^{-1}(x)T_{n-1}^{-1}(x)T_n^{-1}(x)\chi_n(x) \tag{12c}$$

Applying the inverse operation on equation $(11c)$ from the left and substituting equation $(12c)$, together with the entry-boundary transformation

$$\chi_n(0) = T_n(0)T_{n-1}(0)T_{n-2}(0).....T_3(0)T_2(0)T_1(0)\chi(0) \tag{12d}$$

we obtain the approximate solution of equation $(4b)$ in the original frame in the form

$$\chi(x) = U(x)\chi(0) \quad , \quad \chi(x) = \begin{pmatrix} \phi(x) \\ \phi^*(x) \end{pmatrix} \quad , \quad \chi(0) = \begin{pmatrix} \phi(0) \\ \phi^*(0) \end{pmatrix} \tag{12e}$$

where the space evolution operator $U(x)$ in the original frame has been obtained in the form

$$U(x) = T_1^{-1}(x)T_2^{-1}(x)T_3^{-1}(x).....T_{n-1}^{-1}(x)T_n^{-1}(x)U_n(x)T_n(0)T_{n-1}(0).....T_2(0)T_1(0) \quad , \quad n \geq 1 \tag{12f}$$

We recall that the boost operators applied in succession in equations $(12a)$-$(12f)$ alternate between the x-axis and y-axis boosts as explained earlier in the form

$$T_{2j}(x) = e^{\frac{1}{2}\theta_{2j}(x)\sigma_x} \quad ; \quad T_{2j+1}(x) = e^{\frac{1}{2}\theta_{2j+1}(x)\sigma_y} \quad , \quad j = 0, 1, 2, 3, ..., \quad ; \quad \theta_0(x) = 0 \tag{12g}$$

Once $U(x)$ is evaluated explicitly and substituted into equation $(12e)$ to obtain $\phi(x)$, $\phi^*(x)$, the desired general solution of the stationary Schroedinger equation $(1a)$ up to n^{th}-order accuracy follows easily using the definition of the wave function $\psi(x)$ in equation $(3a)$. We observe that the general results we have obtained in equations $(9d)$-$(9f)$, $(10a)$-$(10f)$, $(11d)$-$(11e)$ and $(12e)$-$(12f)$ through factorization and successive boost transformations can be compared with the improved WKB (or phase-integral based) results obtained through various methods of expansion by S L Braunstei [4] and S Winitzki in [7]. The boost transformation procedure developed in the present paper is straightforward and quite effective in providing progressively improving approximate solutions of the semiclassical (WKB) model of the stationary Schroedinger equation $(1a)$.

We illustrate the procedure by presenting explicit results for the zeroth-order and first-order approximations below. The first-order probability density profile in a confining linear potential is plotted to test the accuracy level of the first-order approximate solution.

3.4 Zeroth-order approximation

Up to the zeroth-order approximation, we set

$$n=0\ :\quad q_0(x)=p(x)\quad ;\quad \delta_0(x)=\frac{1}{\hbar}\int_{x_0}^{x}p(x')dx' \tag{13a}$$

$$U_0(x)=e^{-i\delta_0(x)\sigma_z}\ =\ \begin{pmatrix} e^{-i\delta_0(x)} & 0\\ 0 & e^{i\delta_0(x)}\end{pmatrix} \tag{13b}$$

$$T_0^{-1}(x)=I\ =\ T_0(x) \tag{13c}$$

to obtain

$$U(x)=U_0(x)\qquad\Rightarrow\qquad U(x)=\begin{pmatrix} e^{-i\delta_0(x)} & 0\\ 0 & e^{i\delta_0(x)}\end{pmatrix} \tag{13d}$$

which we substitute into equation $(12e)$ to obtain the final result

$$\phi(x)=e^{-i\delta_0(x)}\phi(0)\quad ;\quad \phi^*(x)=e^{i\delta_0(x)}\phi^*(0) \tag{13e}$$

Expressing the entry-boundary complex wave amplitudes $\phi(0)$, $\phi^*(0)$ in the polar form

$$\phi(0)=|\phi(0)|e^{-i\vartheta}\quad ;\quad \phi^*(0)=|\phi(0)|e^{i\vartheta} \tag{13f}$$

in equation $(13e)$ and using the result in the definition of the wave function $\psi(x)$ according to equation $(3a)$ gives the solution of equation $(1a)$ to zeroth-order approximation in the form

$$n=0\ :\quad \psi(x)=\frac{A}{\sqrt{p(x)}}\cos(\frac{1}{\hbar}\int_{x_0}^{x}p(x')dx'+\vartheta)\quad ;\quad A=|\phi(0)| \tag{13g}$$

after substituting $\delta_0(x)$ from equation $(13a)$. We notice that this zeroth-order approximation is exactly the leading order WKB approximation $\psi_{wkb}(x)$ in equation $(1g)$. We observe that for complex $\psi(x)$, the general definitions in equation $(3f)$ and the results obtained in equation $(13e)$ provide the zeroth-order solution in the WKB form presented in equation $(1f)$.

3.5 First-order approximation

Up to the first-order approximation, we set

$$n=1\ :\quad \overline{\xi}_0(x)=\frac{1}{2}w(x)\quad ;\quad q_1(x)=p(x)\sqrt{1-\overline{\xi}_0^2(x)}\quad ;\quad \delta_1(x)=\frac{1}{\hbar}\int_{x_0}^{x}q_1(x')dx' \tag{14a}$$

$$U_1(x)=e^{-i\delta_1(x)\sigma_z}\ =\ \begin{pmatrix} e^{-i\delta_1(x)} & 0\\ 0 & e^{i\delta_1(x)}\end{pmatrix} \tag{14b}$$

$$T_1^{-1}(x)=e^{-\frac{1}{2}\theta_1(x)\sigma_y}=\begin{pmatrix} c_1 & is_1\\ -is_1 & c_1\end{pmatrix}\quad ;\quad T_1(0)=e^{\frac{1}{2}\theta_1(x)\sigma_y}=\begin{pmatrix} \bar{c}_1 & -i\bar{s}_1\\ i\bar{s}_1 & \bar{c}_1\end{pmatrix} \tag{14c}$$

where c_1 , s_1 and corresponding entry-boundary values $\bar{c}_1$, $\bar{s}_1$ are defined according to equation $(7e)$ in the form

$$c_1=\cosh\frac{1}{2}\theta_1(x)\quad ;\quad s_1=\sinh\frac{1}{2}\theta_1(x)\quad ;\quad \bar{c}_1=\cosh\frac{1}{2}\theta_1(0)\quad ;\quad \bar{s}_1=\sinh\frac{1}{2}\theta_1(0) \tag{14d}$$

Using equations $(14b)$-$(14c)$ in equation $(12f)$ for the $n = 1$ case, we obtain the space evolution operator $U(x)$ up to the first-order approximation in the form

$$U(x) = T_1^{-1}(x)U_1(x)T_1(0) \quad \Rightarrow \quad U(x) = \begin{pmatrix} \mu(x) & \nu(x) \\ \nu^*(x) & \mu^*(x) \end{pmatrix} \tag{14e}$$

after introducing complex variables $\mu(x)$ and $\nu(x)$ obtained as

$$\mu(x) = \bar{c}_1 c_1 e^{-\frac{i}{2}\delta_1(x)} - \bar{s}_1 s_1 e^{\frac{i}{2}\delta_1(x)} \quad ; \quad \nu(x) = -i(\bar{s}_1 c_1 e^{-\frac{i}{2}\delta_1(x)} - \bar{c}_1 s_1 e^{\frac{i}{2}\delta_1(x)}) \tag{14f}$$

with complex conjugates $\mu^*(x)$ and $\nu^*(x)$.

Substituting $U(x)$ from equation $(14e)$ into equation $(12e)$ provides the solution to first-order approximation (first accuracy level) in the form

$$\phi(x) = \mu(x)\phi(0) + \nu(x)\phi^*(0) \quad ; \quad \phi^*(x) = \mu^*(x)\phi^*(0) + \nu^*(x)\phi(0) \tag{14g}$$

The general wave function $\psi(x)$ defined in equation $(3a)$ is obtained using $\phi(x)$ and $\phi^*(x)$ from equation $(14g)$ in the reorganized form

$$\psi(x) = \frac{1}{2\sqrt{p(x)}}\{\mu^*(x)\phi^*(0) + \mu(x)\phi(0)\} + \frac{1}{2\sqrt{p(x)}}\{\nu^*(x)\phi(0) + \nu(x)\phi^*(0)\} \tag{15a}$$

which on using the polar form of $\phi(0)$, $\phi^*(0)$ from equation $(13f)$ takes the form

$$\psi(x) = \frac{|\phi(0)|}{2\sqrt{p(x)}}\{(\mu^*(x) + \mu(x) + \nu^*(x) + \nu(x))\cos\vartheta + i(\mu^*(x) - \mu(x) - (\nu^*(x) - \nu(x)))\sin\vartheta\} \tag{15b}$$

The definitions of $\mu(x)$, $\nu(x)$ given in equations $(14f)$ are used to obtain

$$\mu^*(x) + \mu(x) + \nu^*(x) + \nu(x) = 2\{(\bar{c}_1 c_1 - \bar{s}_1 s_1)\cos\delta_1(x) - (\bar{s}_1 c_1 + \bar{c}_1 s_1)\sin\delta_1(x)\} \tag{15c}$$

$$\mu^*(x) - \mu(x) - (\nu^*(x) - \nu(x)) = 2i\{(\bar{c}_1 c_1 + \bar{s}_1 s_1)\sin\delta_1(x) - (\bar{s}_1 c_1 - \bar{c}_1 s_1)\cos\delta_1(x)\} \tag{15d}$$

which we substitute into equation $(15b)$, reorganize and then apply standard trigonometric identities to obtain

$$\psi(x) = \frac{|\overline{\phi}(0)|}{\sqrt{p(x)}}\{\bar{c}(c_1\cos(\delta_1(x)+\vartheta) - s_1\sin(\frac{1}{2}\delta_1(x)+\vartheta)) - \bar{s}(s_1\cos(\delta_1(x)-\vartheta) + c_1\sin(\delta_1(x)-\vartheta))\} \tag{15e}$$

Using the general definition of $\cosh\theta(x)$ in equation $(8c)$, applying the hyperbolic function identities

$$c_1^2 - s_1^2 = 1 \quad ; \quad c_1^2 + s_1^2 = \cosh\theta(x) \quad ; \quad 2c_1 s_1 = \sinh\theta(x) \tag{16a}$$

and introducing appropriately defined parameters $f_+(x)$ and $f_-(x)$ gives

$$c_1 = \frac{f_+(x)}{\left(\sqrt{1 - \overline{\xi}_0^2(x)}\right)^{\frac{1}{2}}} \quad ; \quad s_1 = \frac{f_-(x)}{\left(\sqrt{1 - \overline{\xi}_0^2(x)}\right)^{\frac{1}{2}}} \tag{16b}$$

where

$$f_+(x) = \sqrt{\frac{1}{2}\left(1 + \sqrt{1 - \overline{\xi}_0^2(x)}\right)} \quad ; \quad f_-(x) = \sqrt{\frac{1}{2}\left(1 - \sqrt{1 - \overline{\xi}_0^2(x)}\right)} \tag{16c}$$

Substituting equation (16b) into equation (15e) gives the general wave function in the two-component form

$$\psi(x) = \psi_+(x) - \psi_-(x) \tag{17a}$$

where the components $\psi_+(x)$ and $\psi_-(x)$ have been obtained as

$$\psi_+(x) = \frac{A}{\sqrt{p(x)\sqrt{1-\bar{\xi}_0^2(x)}}}\{f_+(x)\cos(\delta_1(x)+\vartheta) - f_-(x)\sin(\delta_1(x)+\vartheta)\} \quad ; \quad A = \bar{c}\ |\phi(0)| \tag{17b}$$

$$\psi_-(x) = \frac{B}{\sqrt{p(x)\sqrt{1-\bar{\xi}_0^2(x)}}}\{f_-(x)\cos(\delta_1(x)-\vartheta) + f_+(x)\sin(\delta_1(x)-\vartheta)\} \quad ; \quad B = \bar{s}\ |\phi(0)| \tag{17c}$$

with constants A and B defined as shown in the equations. According to the definitions in equation (16b), we obtain

$$\bar{c_1} = \frac{f_+(0)}{\left(\sqrt{1-\bar{\xi}_0^2(0)}\ \right)^{\frac{1}{2}}} \quad ; \quad \bar{s_1} = \frac{f_-(0)}{\left(\sqrt{1-\bar{\xi}_0^2(0)}\ \right)^{\frac{1}{2}}} \tag{17d}$$

The forms of $\psi_+(x)$ and $\psi_-(x)$ in equations (17b) and (17c) suggest that we can introduce a space-dependent phase angle $\varphi(x)$ defined by

$$\cos\varphi(x) = f_+(x) \quad ; \quad \sin\varphi(x) = f_-(x) \tag{17e}$$

which we substitute into equations (17b)-(17c), apply standard trigonometric identities and then substitute the renormalized momentum $q_1(x)$ from equation (14a) to obtain $\psi_+(x)$ and $\psi_-(x)$ in the final forms

$$\psi_+(x) = \frac{A}{\sqrt{q_1(x)}}\cos(\delta_1(x)+\varphi(x)+\vartheta) \quad ; \quad \psi_-(x) = \frac{B}{\sqrt{q_1(x)}}\sin(\delta_1(x)+\varphi(x)-\vartheta) \tag{17f}$$

Substituting the definition of $\delta_1(x)$ from equation (14a) into these results gives the familiar forms

$$\psi_+(x) = \frac{A}{\sqrt{q_1(x)}}\cos(\frac{1}{\hbar}\int_{x_0}^{x} q_1(x')\ dx' + \varphi(x) + \vartheta) \tag{17g}$$

$$\psi_-(x) = \frac{B}{\sqrt{q_1(x)}}\sin(\frac{1}{\hbar}\int_{x_0}^{x} q_1(x')\ dx' + \varphi(x) - \vartheta) \tag{17h}$$

We can reorganize and apply the parameter definitions of c_1 , s_1, $\bar{c}_1$, $\bar{s}_1$ as appropriate to obtain the general wave function in the alternative form

$$\psi(x) = \frac{A}{\sqrt{q_1(x)}}(\cos(\varphi-\vartheta)\cos(\delta_1(x)+\varphi(x)) - \sin(\varphi+\vartheta)\sin(\delta_1(x)+\varphi(x))) \tag{18a}$$

where the constants A and φ have been obtained as

$$A = \frac{|\phi(0)|}{\left(\sqrt{1-\bar{\xi}_0^2(0)}\ \right)^{\frac{1}{2}}} \quad ; \quad \varphi = \varphi(0) \quad \Rightarrow \quad \cos\varphi = f_+(0) \quad , \quad \sin\varphi = f_-(0) \tag{18b}$$

In a simpler case with only one constant parameter-dependent phase angle, we set $\vartheta = \varphi$ in equation (18a) to obtain

$$\vartheta = \varphi: \quad \psi(x) = \frac{A}{\sqrt{q_1(x)}}(\cos(\delta_1(x)+\varphi(x)) - \sin(2\varphi)\sin(\delta_1(x)+\varphi(x))) \tag{18c}$$

3.5.1 The probability density

Since the field potential $V(x)$ is arbitrary, the total energy range includes both the allowed energy region ($E > V(x)$) and the classically forbidden region ($E < V(x)$). The dynamics described by the general wave function obtained in the set of equations (17a)-(17h) or (18a)-(18c) is expected to be normal in the allowed energy region and then change discontinuously as the system approaches the turning point into the classically forbidden region where the fundamental phenomenon of quantum tunneling is expected. The general features of the dynamics over the entire energy range can be studied through the probability density profile.

The probability density to first-order approximation, $\rho_1(x)$, is obtained according to the definition

$$\rho_1(x) = |\bar{\psi}(x)|^2 \;=\; \bar{\psi}_+^2(x) + \bar{\psi}_-^2(x) - 2\bar{\psi}_+(x)\bar{\psi}_-(x) \tag{19a}$$

where

$$\bar{\psi}(x) = \frac{\psi(x)}{A} = \bar{\psi}_+(x) - \bar{\psi}_-(x) \quad ; \quad \bar{\psi}_+(x) = \frac{\psi_+(x)}{A} \quad ; \quad \bar{\psi}_-(x) = \frac{\psi_-(x)}{A} \tag{19b}$$

noting that in dividing $\psi_-(x)$ by A, we obtain

$$\frac{B}{A} = \frac{\bar{s}}{\bar{c}} \;=\; \sqrt{\frac{1-\sqrt{1-\bar{\xi}_0^2(0)}}{1+\sqrt{1-\bar{\xi}_0^2(0)}}} \tag{19c}$$

where we have used the definitions in equations (16c) and (17d), with $\psi_+(x)$, $\psi_-(x)$ in the forms (17b)-(17c) or (17f)-(17h) as convenient. We may also use $\psi(x)$ in the alternative form in equations (18a)-(18c).

3.5.2 The phase accumulation integral

The phase accumulation integral $\delta_1(x)$ defined in equation (14a) can be evaluated exactly or to very good approximation once the field potential $V(x)$ for a given system is specified.

In general, the evaluation of the phase accumulation integral is simplified by obtaining an appropriate binomial expansion of the renormalized momentum $q_1(x)$ using $\bar{\xi}_0(x) = \frac{1}{2}w(x)$ as the expansion parameter. The suitability of $\bar{\xi}_0(x)$ as an expansion parameter follows immediately from the fact that it satisfies the WKB condition ($w(x) \ll 1$) according to equation (1d). In addition, standard trigonometric identities for $\varphi(x)$ using equations (16c) and (17e) give

$$\cos 2\varphi(x) = \sqrt{1-\bar{\xi}_0^2(x)} \quad ; \quad \sin 2\varphi(x) = \bar{\xi}_0(x) \tag{20a}$$

which shows that $\bar{\xi}_0(x)$ must satisfy the trigonometric condition ($|\sin(..)| \leq 1$)

$$|\bar{\xi}_0(x)| \leq 1 \tag{20b}$$

This includes the WKB approximation condition $\bar{\xi}_0(x) = \frac{1}{2}w(x) \ll 1$ for slowly varying potentials $V(x)$.

The expansion procedure is based on the general condition obtained in equation (20b). But this condition cannot apply fully, since the wave function and probability density in the set of equations (17a)-(18c) experience discontinuity at the value $|\bar{\xi}_0(x)| = 1$ where the momentum renormalization factor vanishes according to

$$|\bar{\xi}_0(x)| = 1 \quad \Rightarrow \quad \sqrt{1-\bar{\xi}_0^2(x)} = 0 \quad ; \quad \frac{1}{\sqrt{1-\bar{\xi}_0^2(x)}} = \infty \tag{20c}$$

which may be called the $\overline{\xi}_0(x)$-*discontinuity* condition. It is important to note that the $\overline{\xi}_0(x)$-discontinuity must occur before reaching the energy turning-point ($E = V(x)$), since $\overline{\xi}_0(x) = \frac{1}{2}w(x)$ is indeterminate at the turning point according to the definition of $w(x)$ in equation ($1d$). This feature of a discontinuity occurring just before the turning point is displayed in the probability profiles below.

The $\overline{\xi}_0(x)$-discontinuity condition in equation ($20c$) means that the upper limit $|\overline{\xi}_0(x)| = 1$ in equation ($20b$) must be excluded. The proper dynamical condition for the parameter $\overline{\xi}_0(x)$ then follows from equations ($20b$) and ($20c$) in the general form

$$|\overline{\xi}_0(x)| < 1 \quad ; \quad \overline{\xi}_0^2(x) < 1 \tag{20d}$$

This condition is necessary and sufficient for using $\overline{\xi}_0^2(x)$ as an expansion parameter to expand $\frac{1}{\sqrt{1-\overline{\xi}_0^2(x)}}$ and $\sqrt{1-\overline{\xi}_0^2(x)}$ according to the general binomial expansion

$$(1+y)^m = 1 + \sum_{n=1}^{\infty} \frac{m(m-1)(m-2).....(m-n+1)}{n!}\ y^n \tag{20e}$$

Setting $y = -\overline{\xi}_0^2(x)$, $m = \pm\frac{1}{2}$ in equation ($20e$) and applying the double factorial results

$$(-1)!! = 1 \quad ; \quad (-3)!! = -1 \tag{20f}$$

to include the $n = 0, 1$ terms gives the final forms

$$\frac{1}{\sqrt{1-\overline{\xi}_0^2(x)}} = \sum_{n=0}^{\infty} \frac{(2n-1)!!}{2^n n!}\ \overline{\xi}_0^{2n}(x) \quad ; \quad \sqrt{1-\overline{\xi}_0^2(x)} = \sum_{n=0}^{\infty} \frac{(-1)^{2n-1}(2n-3)!!}{2^n n!}\ \overline{\xi}_0^{2n}(x) \tag{20g}$$

Notice that, if we express

$$\xi_0(x) = \frac{1}{2}\frac{1}{p}\frac{dp}{dx} = \frac{1}{2}\frac{d\ln p}{dx} \quad \Rightarrow \quad \overline{\xi}_0(x) = \frac{1}{2p}\frac{d\ln p}{dx} \tag{20h}$$

then the expansion in equation ($20g$) can be compared with the form of phase-integral expansion obtained by S L Braunstein in [4].

Substituting the expansion for $\sqrt{1-\overline{\xi}_0^2(x)}$ from equation ($20g$) into the renormalized momentum $q_1(x)$ in equation ($14a$), now setting $\overline{\xi}_0(x) = \frac{1}{2}w(x)$, we obtain an expansion for the phase accumulation integral $\delta_1(x)$ defined in equation ($14a$) in the form

$$\delta_1(x) = \sum_{n=0}^{\infty} \frac{(-1)^{2n-1}(2n-3)!!}{2^n n!}\ \frac{1}{\hbar}\int_{x_0}^{x} p(x')(\frac{1}{2}w(x'))^{2n}\ dx' \tag{21a}$$

Using the definition of the momentum from equation ($1b$) gives

$$p(x) = \sqrt{2m(E-V(x))} \quad ; \quad \frac{dp(x)}{dx} = \frac{m}{p(x)}\frac{-dV(x)}{dx} \ = \ \frac{m}{p(x)}F(x) \tag{21b}$$

which is substituted into equation ($1d$) to obtain the WKB approximation parameter $w(x)$ in the form

$$w(x) = \frac{m\hbar}{p^3(x)}\left(-\frac{dV(x)}{dx}\right) \ = \ \frac{m\hbar}{p^3(x)}F(x) \tag{21c}$$

after identifying the classical force $F(x)$ obtained as usual from the field potential $V(x)$ according to

$$F(x) = -\frac{dV(x)}{dx} \tag{21d}$$

From equation (21c) follows (noting $(-1)^{2n} = 1$)

$$(\frac{1}{2}w(x))^{2n} = \left(\frac{m\hbar}{2}\right)^{2n} \frac{1}{p^{6n}(x)} \left(\frac{dV(x)}{dx}\right)^{2n} \quad ; \quad p(x)(\frac{1}{2}w(x))^{2n} = \left(\frac{m\hbar}{2}\right)^{2n} \frac{1}{p^{6n-1}(x)} \left(\frac{dV(x)}{dx}\right)^{2n} \tag{21e}$$

Using equation (21e) in equation (21a) and substituting $p(x) = \sqrt{2m(E - V(x))}$ provides the phase accumulation integral expansion in the final form

$$\delta_1(x) = \sum_{n=0}^{\infty} \frac{(-1)^{2n-1}(2n-3)!!}{2^n n!} \left(\frac{m\hbar}{2}\right)^{2n-1} \int_{x_0}^{x} \frac{m}{\left(\sqrt{2m(E - V(x'))}\right)^{6n-1}} \left(\frac{dV(x')}{dx'}\right)^{2n} dx' \tag{21f}$$

after factoring $m^{2n} = m^{2n-1}m$.

An important point to note is that the phase accumulation integral $\delta_1(x)$ obtained explicitly in terms of the field potential $V(x)$ in equation (21f) is exactly evaluated analytically or using a suitable computer program, e.g., Mathematica, for many different forms of the arbitrary field potential $V(x)$. In some cases, the results are expressed in terms of appropriate special functions. Where the results are too long to be presented in closed form for all n, only a finite number of expansion terms may be used.

3.5.3 Example: probability density profile in a linear potential: $V(x) = \kappa x$

To compare the first-order approximation with the leading order WKB approximation (zeroth-order approximation) displayed in Fig. 1, we evaluate the first-order probability density $\rho_1(x)$ defined in equation (18a) for the case of the linear potential $V(x) = \kappa x$ and display the profile in Fig. 2 below. The evaluations are simplified for any mass m , mean total energy E and field potential coupling constant κ using the potential and parameter definitions given in equation (1i).

We have discovered that for $\vartheta = \pm\frac{\pi}{4}$, the probability density $\rho_1(x)$ in equation (19a) takes infinite values according to

$$\rho_1(x \ , \ \vartheta = \mp\frac{\pi}{4}) = \pm\infty \tag{22a}$$

which means that for entry-boundary values $\vartheta = \mp\frac{\pi}{4}$, the dynamics in a linear potential is *indeterminate* even in the allowed energy region $E \geq \kappa x$. Noting that the behavior is very highly sensitive to the entry-boundary values, we choose ϑ arbitrarily close to $\frac{\pi}{4}$ to compare $\rho_1(x)$ from equation (19a) with the WKB leading order probability density $\rho_{wkb}(x)$ in equation (1h) displayed in Fig. 1.

The probability density profile from equation (19a) for dynamics in a linear field potential $V = \kappa x$ is displayed in Fig. 2 for entry-boundary phase angle $\vartheta = (1 \pm 10^{-10})\frac{\pi}{4} \equiv \frac{\pi}{4}$, which we have chosen to be arbitrarily close to the WKB asymptotic value $\vartheta = \frac{\pi}{4}$ in equation (1g). We have used the expansion in equation (21f) to include $n = 0 \rightarrow 50000$ exactly evaluated terms so that the phase accumulation integral $\delta_1(x)$ is essentially exact.

$$\rho_1(x) \;\; \text{for} \;\; V(x) = \kappa x \quad , \quad p(x) = \sqrt{b - ax} \quad , \quad b = 2mE \; , \; a = 2m\kappa \quad ; \quad \vartheta = (1 \pm 10^{-10})\frac{\pi}{4} \equiv \frac{\pi}{4} \tag{22b}$$

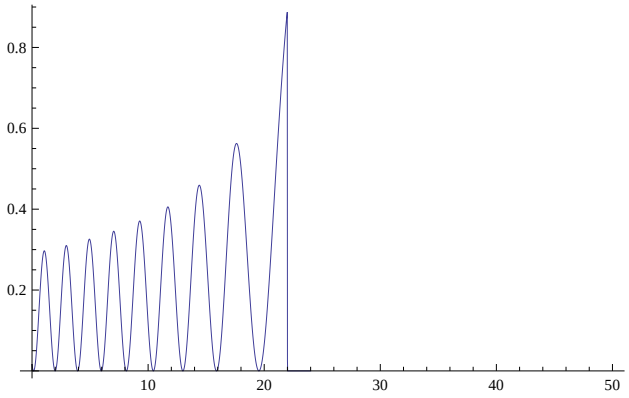

Figure 2: First-order probability density $\rho_1(x)$ for linear potential $V(x) = \kappa x$ with $b = 12$, $a = 0.5$, $\vartheta \equiv \frac{\pi}{4}$ over the range $x = 0 \to 50$

.

This diagram clearly reveals a rapid increase, like a discontinuity, in the probability density at the turning point, followed immediately by a rapid collapse to zero. The probability density $\rho_1(x)$ remains exactly zero throughout the region beyond the turning point, which reveals that the particle is confined within the allowed energy region $E > \kappa x$. This confirms the well known confining property of the linear potential $V(x) = \kappa x$. In contrast, the leading order WKB probability density $\rho_{wkb}(x)$ in equation $(1h)$ displayed in Fig. 1 undergoes a discontinuous change, increasing very sharply near the turning point and remains indeterminate beyond the turning point. The leading order WKB approximation does not tell what happens to the particle once it gets close to the turning point and thus fails to reveal the confining property of the linear potential. The first-order approximate solution obtained through the factorization and boost transformation presented in final form in equations $(17a)$-$(17h)$ or $(18a)$-$(18c)$ is therefore much more accurate compared to the leading order WKB approximation presented in equations $(1f)$-$(1g)$.

4 Space-dependent spin / polarization state vectors

An important outcome of the matrix method is the emergence of the basic spin or polarization state vectors in the definition of χ according to

$$\chi = \phi \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \phi^* \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad \Rightarrow \quad \chi(x) = \phi(x)|0\rangle + \phi^*(x)|1\rangle \quad ; \quad \chi(0) = \phi(0)|0\rangle + \phi^*(0)|1\rangle \tag{23a}$$

where we have recognized the basic spin state vectors $|0\rangle$ and $|1\rangle$ defined by

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad ; \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{23b}$$

Substituting $\chi(0)$ from equation $(23a)$ into equation $(12e)$, we obtain

$$\chi(x) = U(x)\chi(0) = \phi(0)|0; x\rangle + \phi^*(0)|1; x\rangle \tag{23c}$$

where we have introduced space-dependent spin / polarization state vectors $|0;x\rangle$, $|1;x\rangle$ obtained according to

$$|0;x\rangle = U(x)|0\rangle \quad ; \quad |1;x\rangle = U(x)|1\rangle \tag{23d}$$

Noting that polarization states are specified as positive $(+)$ and negative $(-)$ helicity states, we introduce appropriate notation for polarization state vectors according to

$$|+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad ; \quad |-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{23e}$$

The space-dependent positive and negative helicity polarization state vectors are obtained as

$$|+;x\rangle = U(x)|+\rangle \quad ; \quad |-;x\rangle = U(x)|-\rangle \tag{23f}$$

We introduce spin / polarization operators

$$\hat{S}_0 = \frac{\hbar}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|) \quad ; \quad \hat{S}_z = \frac{\hbar}{2}(|0\rangle\langle 0| - |1\rangle\langle 1|) \tag{24a}$$

$$\hat{S}_x = \frac{\hbar}{2}(|0\rangle\langle 1| + |1\rangle\langle 0|) \quad ; \quad \hat{S}_y = -\frac{i\hbar}{2}(|0\rangle\langle 1| - |1\rangle\langle 0|) \tag{24b}$$

Spin / polarization states are described by the mean values of these operators obtained as

$$S_j = \chi^\dagger(x)\hat{S}_j\chi(x) = \chi^\dagger(0)U^{-1}(x)\hat{S}_jU(x)\chi(0) \quad ; \quad j = 0, x, y, z \tag{24c}$$

where

$$\chi^\dagger(x) = \chi^\dagger(0)U^{-1}(x) \quad ; \quad \chi^\dagger(0) = \phi^*(0)\langle 0| + \phi(0)\langle 1| \tag{24d}$$

The mean parameters S_j can be used to determine the distribution of the spin / polarization states on appropriately defined geometric surfaces in the semiclassical model of the stationary Schroedinger equation $(1a)$. Details will be presented in another paper.

5 Conclusion

We have provided a general approximate solution of arbitrary level of accuracy of the semiclassical model of the stationary Schroedinger equation through factorization and successive boost transformations of the equivalent matrix equation. The fact that the basic approximation parameter, starting with the zeroth-order parameter $\xi_0(x) = \frac{\hbar}{2p(x)}\frac{dp(x)}{dx}$, reduces progressively under successive boost operations from dynamical frames of lower accuracy to dynamical frames of higher accuracy has led to the concept of accuracy levels. Each dynamical frame represents an accuracy level and an advancement from a frame of lower accuracy level to a frame of higher accuracy level is achieved through a boost transformation or an appropriate succession of boost transformations. A boost transformation operator, $T(x)$, thus provides a mechanism, i.e., a theoretical tool, for improving the accuracy of an approximation. We have demonstrated in equations $(10a)$-$(10f)$ that the boost transformations effectively generate series expansions in terms of derivatives of progressively increasing order of the basic approximation parameter $\overline{\xi}_0(x) = \frac{\xi_0(x)}{p(x)} = \frac{1}{2}w(x)$, where $w(x)$ is the usual WKB approximation parameter, sometimes called the adiabatic parameter. The boost transformation procedure is more elegant compared to perturbation and other expansion methods which are generally tedious.

In the general solution procedure developed in the present paper, the original frame (normally identified as the laboratory frame) where the stationary Schroedinger equation $(1a)$ is specified is

classified as the zeroth-order approximation or lowest accuracy dynamical frame. We have established that the zeroth-order approximation provides the leading order WKB-approximation, which is exact in a constant potential where the momentum p is constant. The first-order and higher-order approximations provide progressively more accurate solutions.

The general solutions obtained in this paper apply to all types of second-order ordinary differential equations similar to the Schroedinger equation, which are generally expressed in the form of equation $(1c)$ in mathematics, physics, chemistry, biology, economics and other disciplines where such second-order processes occur. In the general cases, a suitable expansion parameter is introduced to replace the quantization parameter $\hbar$ which occurs in the Schroedinger equation. If the function ψ in the equation equivalent to $(1a)$ is complex, then the general solution is obtained in terms of the components $\phi \to \phi_-$ and $\phi_* \to \phi_+$ defined according to equations $(3a)$ and $(3f)$.

The space-dependent spin / polarization state vectors introduced here will prove very useful in describing the stationary quantum states of a system in the semiclassical model, as we will demonstrate in a future paper.

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