WKB Approximation in Two Dimensions

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(abstract)

1. SEPARATION OF VARIABLES IN 2D CARTESIAN COORDINATES

In two dimensions (2D) the time independent Schrödinger equation becomes

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)\psi(x,y)+V(x,y)\psi(x,y) = E\psi(x,y), \tag{1}$$

where $V(x,y)$ is a 2D potential. We'll assume that the solution is the product of separate functions in x and y:

$$\psi(x,y) = X(x)Y(y). \tag{2}$$

The 2D Schrödinger equation can be separated into two ordinary differential equations (ODE) if the potential can be written as a sum of x and y components:

$$V(x,y) = V_x(x) + V_y(y). \tag{3}$$

Substituting these definitions from equations (2,3) into the 2D Schrödinger equation (1), we have

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)X(x)Y(y) + \left(V_x(x)+V_y(y)\right)X(x)Y(y) = EX(x)Y(y). \tag{4}$$

Then, distributing the derivatives and the separated potential results in

$$\left[-\frac{\hbar^2}{2m}Y(y)\frac{d^2X(x)}{dx^2}+V_x(x)X(x)Y(y)\right] + \left[-\frac{\hbar^2}{2m}X(x)\frac{d^2Y(y)}{dy^2}+V_y(x)X(x)Y(y)\right] = EX(x)Y(y). \tag{5}$$

And after dividing by $X(x)Y(y)$, we are left with

$$E = \left[-\frac{\hbar^2}{2m}\frac{1}{X(x)}\frac{d^2X(x)}{dx^2}+V_x(x)\right] + \left[-\frac{\hbar^2}{2m}\frac{1}{Y(y)}\frac{d^2Y(y)}{dy^2}+V_y(x)\right]. \tag{6}$$

The first term is a function of x only, while the second term depends only on y. Also, E is constant over x and y. Therefore the first two terms are each a constant:

$$E_x = -\frac{\hbar^2}{2m}\frac{1}{X(x)}\frac{d^2X(x)}{dx^2}+V_x(x) \tag{7a}$$

$$E_y = -\frac{\hbar^2}{2m}\frac{1}{Y(y)}\frac{d^2Y(y)}{dy^2}+V_y(x) \tag{7b}$$

$$E = E_x + E_y \tag{7c}$$

2. EXAMPLE 1: 2D FINITE BARRIER IN AN INFINITE SQUARE WELL

We can imagine a 2D system, that has a finite barrier in both x and y as shown in figure ¡fig 1¿ as its potential. The total potential is the sum of the two:

$$V(x,y) = V_x(x) + V_y(y) \tag{8}$$

We'll start by finding the wavefunctions in the x-dimension.

2.1. $E < V_0$

When the total energy is less than the potential barrier the wavefunction is sinusiodal on either side. Within the barrier it exponentially decays approaching the center.

2.1.1. *Region* α $(-d_1 < x < 0)$

In region *alpha*, where $V = 0$, the Schrödinger equation becomes

$$\frac{d^2}{dx^2}\psi(x) + \frac{2mE}{\hbar^2}\psi(x) = 0, \tag{9}$$

and the general solution is

$$\psi(x) = Ae^{ikx} + A_0e^{-ikx}, \tag{10a}$$

where

$$k = \sqrt{2mE}/\hbar. \tag{10b}$$

However at $x = -d_1$, $|\psi(x)^2| = 0$. Therefore,

$$A_0 = \frac{-Ae^{ikd_1}}{e^{-ikd_1}} = -Ae^{2ikd_1}. \tag{11}$$

Finally, the wavefunction in region α is

$$\psi_\alpha(x) = A[e^{ikx} - e^{2ikd_1}e^{-ikx}] \tag{12}$$

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2.1.2. Region β ($0 < x < d_2$)

In region β, $V(x) = V_0$ and the Schrödinger equation becomes

$$\frac{d^2}{dx^2}\psi(x) - \frac{2m}{\hbar^2}(V_0 - E)\psi(x) = 0, \tag{13}$$

and the general solution is

$$\psi_\beta(x) = Be^{nx} + Ce^{-nx}, \tag{14a}$$

where

$$n = \frac{\sqrt{2m(V_0 - E)}}{\hbar} \tag{14b}$$

2.1.3. Region γ ($d_2 < x < d_2 + d_3$)

In region γ where $V = 0$, the general solution is the same as (10), but we'll designate different constants:

$$\psi_\gamma(x) = De^{ikx} + D_0 e^{-ikx}, \tag{15a}$$

where again

$$k = \sqrt{2mE}/\hbar. \tag{15b}$$

At the right boundary of the well, the wavefunction must be zero: $|\psi(d_2 + d_3)|^2 = 0$. Thus

$$D_0 = -D\frac{e^{ik(d_2+d_3)}}{e^{-ik(d_2+d_3)}} = -De^{2ik(d_2+d_3)}, \tag{16}$$

and finally the wavefunction becomes

$$\psi_\gamma(x) = D[e^{ikx} - e^{2ik(d_2+d_3)}e^{-ikx}]. \tag{17}$$

2.1.4. Boundary Conditions Between Regions

Additional boundary conditions can be imposed between the three regions. This will lead to the eigenvalues and eventually, to solving for the constants. The wavefunction and its derivative must be continuous at the boundaries.

Equating the the wavefunctions at the boundary of the α region and β region:

$$A[e^{ikx} - e^{2ikd_1}e^{-ikx}]|_{x=0} = [Be^{nx} + Ce^{-nx}]|_{x=0}, \tag{18}$$

thus

$$A[1 - e^{2ikd_1}] = B + C. \tag{19}$$

And equating the derivatives at the boundary:

$$A[ike^{ikx} + ike^{2ikd_1}e^{-ikx}]|_{x=0} = [Bne^{nx} - Cne^{-nx}]|_{x=0}, \tag{20}$$

therefore,

$$iAk[1 + e^{2ikd_1}] = Bn - Cn. \tag{21}$$

Equating the wavefunctions at the boundary of the β-region and the γ-region ($x = d_2$), leads to

$$Be^{nd_2} + Ce^{-nd_2} = D[e^{ikd_2} - e^{2ik(d_2+d_3)}e^{-ikd_2}]. \tag{22}$$

And by equating the derivatives between the β- and γ-regions,

$$Bne^{nd_2} - Cne^{-nd_2} = D[ike^{ikd_2} + ike^{2ik(d_2+d_3)}e^{-ikd_2}]. \tag{23}$$

We can combine equations (19, 21, 22, 23) into a matrix equation:

$$\mathbf{M}\begin{pmatrix} A \\ B \\ C \\ D \end{pmatrix} = \mathbf{0}$$

$$= \begin{pmatrix} 1 - e^{2ikd_1} & -1 & -1 & 0 \\ ik[1 + e^{2ikd_1}] & -n & n & 0 \\ 0 & e^{nd_2} & e^{-nd_2} & e^{ikd_2} - f \\ 0 & ne^{nd_2} & -ne^{-nd_2} & ik[e^{ikd_2} + f] \end{pmatrix}\begin{pmatrix} A \\ B \\ C \\ D \end{pmatrix} \tag{24a}$$

where

$$f = e^{2ik(d_2+d_3)}e^{-ikd_2}. \tag{24b}$$

And then the Eigenvalues can be found from the following determinant:

$$\begin{vmatrix} 1 - e^{2ikd_1} & -1 & -1 & 0 \\ ik[1 + e^{2ikd_1}] & -n & n & 0 \\ 0 & e^{nd_2} & e^{-nd_2} & e^{ikd_2} - f \\ 0 & ne^{nd_2} & -ne^{-nd_2} & ik[e^{ikd_2} + f] \end{vmatrix} = 0. \tag{25}$$

Evaluating the determinant, and grouping like terms leaves us with

$$\begin{aligned} &(1 - e^{2ikd_1})\big[-ikn(e^{nd_2} + e^{-nd_2})(e^{ikd_2} + f) \\ &\qquad + n^2(e^{nd_2} - e^{-nd_2})(e^{ikd_2} - f)\big] \\ &+ ik(1 + e^{2ikd_1})\big[ik(e^{-nd_2} - e^{nd_2})(e^{ikd_2} + f) \\ &\qquad + n(e^{nd_2} + e^{-nd_2})(e^{ikd_2} - f)\big] = 0. \end{aligned} \tag{26}$$

After substituting in equation (24b), and replacing some exponentials with trigonometric and hyperbolic functions, we have

$$\begin{aligned} &\tan(kd_1)\big[-2ikn(\cosh(nd_2))[e^{2ikd_2} + e^{2ik(d_2+d_3)}] \\ &\qquad + 2n^2\sinh(nd_2)[e^{2ikd_2} - e^{2ik(d_2+d_3)}]\big] \\ &+k\big[-2ik\sinh(nd_2)[e^{2ikd_2} + e^{2ik(d_2+d_3)}] \\ &\qquad + 2n\cosh(nd_2)[e^{2ikd_2} - e^{2ik(d_2+d_3)}]\big] = 0. \end{aligned} \tag{27}$$

By dividing by e^{2ikd_2}, and factoring out the $(1 - e^{2ikd_3})$ and $i(1 + e^{2ikd_3})$ terms:

$$
\begin{aligned}
&i(1 + e^{2ikd_3})\big[2kn\cosh(nd_2)\tan(kd_1) + 2k^2\sinh(nd_2)\big] \\
&= (1 - e^{2ikd_3})\big[2n^2\sinh(nd_2)\tan(k_d 1) + 2nk\cosh(nd_2)\big].
\end{aligned}
\tag{28}
$$

The quotient of the aforementioned terms is $\tan(kd_3)$, and we can divide by $\cosh(nd_2)$. Finally, the condition for eigenvalues when $E < V_0$ is

$$
\begin{aligned}
&kn\tan(kd_1) + k^2\tanh(nd_2) \\
&= \tan(kd_3)\big[n^2\tanh(nd_2)\tan(kd_1) + kn\big].
\end{aligned}
\tag{29}
$$