Howard University
Washington, DC 20059

Department of Physics and Astronomy
(202)-806-6245 (Main Office)
(202)-806-5830 (fax)

2355 Sixth St., NW, TKH Rm.215
thubsch@howard.edu
(202)-806-6257

Quantum Mechanics II
Case Studies

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Handout (T. Hübsch)

1. WKB: Wells and Barriers

Consider the 1-dimensional Schrödinger equation for stationary states:

$$\Big[-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}+V(x)\Big]\psi_{_E}(x)=E\psi_{_E}(x)\ . \tag{1.1}$$

1.1. The solutions

Substituting $\psi_E(x)=e^{iu(x)}$, where $u(x)$ a complex function, produces

$$(u')^2=k^2+iu''\ ,\qquad\text{where}\qquad k(x)\stackrel{\text{def}}{=}+\sqrt{\frac{2m}{\hbar^2}\big[E-V(x)\big]}\ , \tag{1.2}$$

which is a non-linear equation. It can be solved iteratively, starting with the assumption that $u''\ll(u')^2-k^2$; this defines the 0^{th} order solution:

$$u_0'=\pm k(x)\ ,\qquad\text{so}\qquad u(x)=\pm\int\mathrm{d}x\ k(x)+C_0\ ,$$

where C_0 is the constant of integration. The solution to the nonlinear differential equation (1.2) is then approached by iteratively calculating, for $n=1,2,3,\ldots$:

$$u_n'=\pm\sqrt{k^2+iu_{n-1}''}\ ,\qquad\text{so}\qquad u_n(x)=\pm\int\mathrm{d}x\ \sqrt{k^2(x)+iu_{n-1}''(x)}+C_n\ .$$

The exact solution is then $u(x)=\lim_{n\to\infty}u_n(x)$, and we obviously must stop at a finite n for this to be feasible at all.

As it turns out, already $n=1$ (the WKB approximation) gives a pretty good approximation:

$$\begin{aligned}
u_1(x)&=\pm\int\mathrm{d}x\ \sqrt{k^2(x)+iu_0''(x)}+C_1=\pm\int\mathrm{d}x\ \sqrt{k^2(x)\pm ik'(x)}+C_1\ ,\\
&=\pm\int\mathrm{d}x\ k(x)\sqrt{1\pm\frac{ik'(x)}{k^2(x)}}+C_1=\pm\int\mathrm{d}x\ k(x)\Big(1\pm\frac{ik'(x)}{2k^2(x)}+\ldots\Big)+C_1\ ,\\
&=\pm\int\mathrm{d}x\ k(x)+\tfrac{i}{2}\int\mathrm{d}x\ \frac{k'(x)}{k(x)}+\ldots+C_1\ ,\\
&=\pm\int\mathrm{d}x\ k(x)+\tfrac{i}{2}\log[k(x)]+\ldots+C_1\ .
\end{aligned}$$

At this point, we drop the ellipses reminding us of the dropped terms in the expansion of the square-root, and express the integration constant as the value of the given integral at some suitable reference point, x_*, so that

$$u_1(x) = \pm \int_{x_*}^{x} \mathrm{d}\xi\ k(\xi) + \tfrac{i}{2}\log[k(x)]\ ,$$

that is, since there are the two solutions with the two signs:

$$\psi_E^{(1)}(x) = e^{iu_1(x)} = \frac{A}{\sqrt{k(x)}} e^{i\int_{x_*}^{x} \mathrm{d}x\, k(x)} + \frac{B}{\sqrt{k(x)}} e^{-i\int_{x_*}^{x} \mathrm{d}x\, k(x)} \tag{1.3a}$$

This is called the WKB solution. For the classically forbidden region, where $V(x) > E$, we write $k(x) = i\kappa(x) \stackrel{\text{def}}{=} +i\sqrt{2m[V(x)-E]}/\hbar$, and obtain

$$\psi_E^{(1)}(x) = e^{iu_1(x)} = \frac{C}{\sqrt{k(x)}} e^{-\int_{x_*}^{x} \mathrm{d}x\, \kappa(x)} + \frac{D}{\sqrt{k(x)}} e^{+\int_{x_*}^{x} \mathrm{d}x\, \kappa(x)}\ . \tag{1.3b}$$

1.2. Matching conditions

As described in detail in Ref. [6], and presented in Ref. [9], the two types of solutions can be matched across as follows:

1 **If $V(x)$ crosses E discontinuously:**
one must use $\psi(x_*{+}0^+) = \psi(x_*{+}0^-)$ and $\psi'(x_*{+}0^+) = \psi'(x_*{+}0^-)$.
Note: $f(x_*{+}0^\pm) \stackrel{\text{def}}{=} \lim_{\epsilon\to 0} f(x_*{\pm}\epsilon)$, with $\epsilon \geq 0$.

2 **If $V(x)$ crosses E discontinuously:**
one must use the following identifications:

2.a *the barrier (classically forbidden region) to the left*:

$$C = (\vartheta^* A{+}\vartheta B)\ , \quad D = \tfrac{1}{2}(\vartheta A{+}\vartheta^* B)\ ; \qquad A = \tfrac{1}{2}\vartheta C{+}\vartheta^* D\ , \quad B = \tfrac{1}{2}\vartheta^* C{+}\vartheta D\ .$$

2.b *the barrier (classically forbidden region) to the left*:

$$C = \tfrac{1}{2}(\vartheta^* A{+}\vartheta B)\ , \quad D = (\vartheta A{+}\vartheta^* B)\ ; \qquad A = \vartheta C{+}\tfrac{1}{2}\vartheta^* D\ , \quad B = \vartheta^* C{+}\tfrac{1}{2}\vartheta D\ .$$

Here $\vartheta = e^{i\pi/4}$ and $\vartheta^* = e^{-i\pi/4}$ are the phases imparted on the amplitudes by the WKB matching conditions.

1.3. Potential well

Consider a $V(x)$, defined over $x \in (-\infty, +\infty)$, such that $V(x) < E$ for $x \in (x_a, x_b)$, but $V(x) > E$ outside the $[x_a, x_b]$ interval. The WKB wave-function is then:

$$\psi(x) = \begin{cases} \frac{C}{\sqrt{\kappa(x)}} e^{-\int_{x_a}^{x} \mathrm{d}\xi\, \kappa(\xi)} + \frac{D}{\sqrt{\kappa(x)}} e^{+\int_{x_a}^{x} \mathrm{d}\xi\, \kappa(\xi)}\ , & \text{I: for } x < x_a, \\[2mm] \frac{A}{\sqrt{k(x)}} e^{i\int_{x_a}^{x} \mathrm{d}\xi\, k(\xi)} + \frac{B}{\sqrt{k(x)}} e^{-i\int_{x_a}^{x} \mathrm{d}\xi\, k(\xi)}\ , & \text{II: for } x_a < x < x_b, \\[2mm] \frac{C'}{\sqrt{\kappa(x)}} e^{-\int_{x_b}^{x} \mathrm{d}\xi\, \kappa(\xi)} + \frac{D'}{\sqrt{\kappa(x)}} e^{+\int_{x_b}^{x} \mathrm{d}\xi\, \kappa(\xi)}\ , & \text{III: for } x > x_b, \end{cases}$$

where the constants in the third region are distinguished from those in the first one by the prime. The reference points for wave-functions in the "external" regions have been chosen to refer to the nearest classical turning point (as that's the point around which the above matching conditions apply). In the middle region, the function can be written with respect to either reference point—but once it is chosen (x_a above), it cannot be changed arbitrarily. This is because the potential $V(x)$, and so the wave number $k(x)$, and therefore also the relative phase between the "A" and "B" components changes with x. we shall see that this change is essential.

We note that $\int_{x_a}^{x} \mathrm{d}x\, \kappa(x) < 0$ in region I, since $x < x_a$ there. Thus, the "C" partial wave diverges for $x \to -\infty$, and we must discard this partial wave to obtain a normalizable function; set $C = 0$.

To apply the matching conditions, we first note that the transition I→II is as described above in 2.a. Therefore, with $C = 0$, we have that

$$\psi(x) = \begin{cases} \frac{D}{\sqrt{\kappa(x)}} e^{+\int_{x_a}^{x} \mathrm{d}\xi\, \kappa(\xi)} \,, & \text{I,} \\ \frac{\vartheta^* D}{\sqrt{k(x)}} e^{i\int_{x_a}^{x} \mathrm{d}\xi\, k(\xi)} + \frac{\vartheta D}{\sqrt{k(x)}} e^{-i\int_{x_a}^{x} \mathrm{d}\xi\, k(\xi)} \,, & \text{II,} \\ \frac{C'}{\sqrt{\kappa(x)}} e^{-\int_{x_b}^{x} \mathrm{d}\xi\, \kappa(\xi)} + \frac{D'}{\sqrt{\kappa(x)}} e^{+\int_{x_b}^{x} \mathrm{d}\xi\, \kappa(\xi)} \,, & \text{III.} \end{cases}$$

To apply the matching condition for the transition II→III (as described in 2.b), we must first shift the reference point of the integrals in region II from $x_a \to x_b$, by writing

$$\int_{x_a}^{x} \mathrm{d}\xi\, k(\xi) = \phi + \int_{x_b}^{x} \mathrm{d}\xi\, k(\xi) \,, \qquad \text{where} \qquad \phi \overset{\text{def}}{=} \int_{x_a}^{x_b} \mathrm{d}\xi\, k(\xi) \,.$$

Then

$$\psi(x) = \begin{cases} \frac{D}{\sqrt{\kappa(x)}} e^{+\int_{x_a}^{x} \mathrm{d}\xi\, \kappa(\xi)} \,, & \text{I,} \\ \frac{\vartheta^* e^{i\phi} D}{\sqrt{k(x)}} e^{i\int_{x_b}^{x} \mathrm{d}\xi\, k(\xi)} + \frac{\vartheta e^{-i\phi} D}{\sqrt{k(x)}} e^{-i\int_{x_b}^{x} \mathrm{d}\xi\, k(\xi)} \,, & \text{II,} \\ \frac{C'}{\sqrt{\kappa(x)}} e^{-\int_{x_b}^{x} \mathrm{d}\xi\, \kappa(\xi)} + \frac{D'}{\sqrt{\kappa(x)}} e^{+\int_{x_b}^{x} \mathrm{d}\xi\, \kappa(\xi)} \,, & \text{III.} \end{cases}$$

Note that $\vartheta^* e^{i\phi} = e^{-i\pi/4} e^{i\phi} = e^{i(\phi-\pi/4)}$ and $\vartheta e^{-i\phi} = e^{-i(\phi-\pi/4)}$. Using this and the matching conditions 2.b, we obtain:

$$\begin{aligned} C' &= (\vartheta^* A + \vartheta B)/2 = [\vartheta^*(\vartheta^* e^{i\phi} D) + \vartheta(\vartheta e^{-i\phi} D)]/2 \\ &= D[e^{i(\phi-\pi/2)} + e^{-i(\phi-\pi/2)}]/2 = D\cos(\phi-\pi/2) = D\sin(\phi), \\ D' &= (\vartheta A + \vartheta^* B) = [\vartheta(\vartheta^* e^{i\phi} D) + \vartheta^*(\vartheta e^{-i\phi} D)] \\ &= D[e^{i\phi} + e^{-i\phi}] = 2D\cos(\phi), \end{aligned}$$

Finally, since the "D'" partial wave diverges for $x \to +\infty$, we must set $D' = 2D\cos(\phi) = 0$, which requires

$$\int_{x_a}^{x_b} \mathrm{d}\xi\, k(\xi) = \int_{x_a}^{x_b} \mathrm{d}\xi \sqrt{\frac{2m}{\hbar^2}\big[E_n - V(\xi)\big]} = (2n+1)\tfrac{\pi}{2} \ .$$

This is the equation that determines the values of energy, E_n, for which there exist bound states, *i.e.*, the discrete part of the spectrum of the Hamiltonian.

1.4. Potential barrier

Consider now the opposite problem, where $V(x)$, defined over $x \in (-\infty, +\infty)$, such that $V(x) > E$ poses a barrier for $x \in (x_a, x_b)$, but $V(x) < E$ outside the $[x_a, x_b]$ interval. The WKB wave-function is then:

$$\psi(x) = \begin{cases} \frac{A}{\sqrt{k(x)}} e^{i\int_{x_a}^{x} \mathrm{d}\xi\, k(\xi)} + \frac{B}{\sqrt{k(x)}} e^{+\int_{x_a}^{x} \mathrm{d}\xi\, k(\xi)} \ , & \text{I: for } x < x_a, \\ \frac{C}{\sqrt{\kappa(x)}} e^{-\int_{x_a}^{x} \mathrm{d}\xi\, \kappa(\xi)} + \frac{D}{\sqrt{\kappa(x)}} e^{+\int_{x_a}^{x} \mathrm{d}\xi\, \kappa(\xi)} \ , & \text{II: for } x_a < x < x_b, \\ \frac{A'}{\sqrt{k(x)}} e^{-\int_{x_b}^{x} \mathrm{d}\xi\, k(\xi)} + \frac{D'}{\sqrt{k(x)}} e^{+\int_{x_b}^{x} \mathrm{d}\xi\, k(\xi)} \ , & \text{III: for } x > x_b, \end{cases}$$

where the constants in the third region are again distinguished from those in the first one by the prime. For future use, we define

$$\sigma \stackrel{\text{def}}{=} \int_{x_a}^{x_b} \mathrm{d}\xi\ \kappa(\xi) \ ,$$

and for the time being leave all the constants in the "outer" regions undetermined. The goal will be to express (A', B') in terms of (A, B) or (A', B) in terms of (B', A). That is, we seek to determine the matrices in the equations:

$$\begin{bmatrix} A' \\ B' \end{bmatrix} = \mathbf{P} \begin{bmatrix} A \\ B \end{bmatrix} \ , \qquad \text{and} \qquad \begin{bmatrix} A' \\ B \end{bmatrix} = \mathbf{S} \begin{bmatrix} A \\ B' \end{bmatrix} \ .$$

These are, indeed, the (propagation) **P**-matrix, describing the I→III propagation of the wave-function, and the (scattering) **S**-matrix, describing the out-going waves, with amplitudes (A', B), in terms of the in-going ones, with amplitudes (A, B').

This time, for the transition I→II we must use the matching conditions 2.b, obtaining

$$\psi(x) = \begin{cases} \frac{A}{\sqrt{k(x)}} e^{i\int_{x_a}^{x} \mathrm{d}\xi\, k(\xi)} + \frac{B}{\sqrt{k(x)}} e^{+\int_{x_a}^{x} \mathrm{d}\xi\, k(\xi)} \ , & \text{I}, \\ \frac{(\vartheta^* A + \vartheta B)e^{-\sigma}}{2\sqrt{\kappa(x)}}\, e^{-\int_{x_b}^{x} \mathrm{d}\xi\, \kappa(\xi)} + \frac{(\vartheta A + \vartheta^* B)e^{\sigma}}{\sqrt{\kappa(x)}}\, e^{+\int_{x_b}^{x} \mathrm{d}\xi\, \kappa(\xi)} \ , & \text{II}, \\ \frac{A'}{\sqrt{k(x)}} e^{-\int_{x_b}^{x} \mathrm{d}\xi\, k(\xi)} + \frac{D'}{\sqrt{k(x)}} e^{+\int_{x_b}^{x} \mathrm{d}\xi\, k(\xi)} \ , & \text{III}, \end{cases}$$

where we have already shifted the integrals in the exponents in region II, and extracted the $e^{\pm\sigma}$ factor. Note that this now is a real boosting/attenuating factor rather than a phase.

Using the matching conditions 2.a for the II→III transition, we finally obtain

$$\psi(x)=\begin{cases}\frac{A}{\sqrt{k(x)}}e^{i\int_{x_a}^{x}\mathrm{d}\xi\,k(\xi)}+\frac{B}{\sqrt{k(x)}}e^{+\int_{x_a}^{x}\mathrm{d}\xi\,k(\xi)}\;, & \text{I},\\ \frac{(\vartheta^*A+\vartheta B)e^{-\sigma}}{2\sqrt{\kappa(x)}}e^{-\int_{x_b}^{x}\mathrm{d}\xi\,\kappa(\xi)}+\frac{(\vartheta A+\vartheta^*B)e^{\sigma}}{\sqrt{\kappa(x)}}e^{+\int_{x_b}^{x}\mathrm{d}\xi\,\kappa(\xi)}\;, & \text{II},\\ \frac{\frac14(A+iB)e^{-\sigma}+(A-iB)e^{\sigma}}{\sqrt{k(x)}}e^{-\int_{x_b}^{x}\mathrm{d}\xi\,k(\xi)}-i\frac{\frac14(A+iB)e^{-\sigma}-(A-iB)e^{\sigma}}{\sqrt{k(x)}}e^{+\int_{x_b}^{x}\mathrm{d}\xi\,k(\xi)}\;, & \text{III}.\end{cases}$$

Thus,

$$\begin{aligned}A'&=(e^{\sigma}+\tfrac14e^{-\sigma})A-i(e^{\sigma}-\tfrac14e^{-\sigma})B\;,\\ B'&=i(e^{\sigma}-\tfrac14e^{-\sigma})A+(e^{\sigma}+\tfrac14e^{-\sigma})B\;.\end{aligned}\tag{1.4}$$

That is (cf. Ref. [8], p.126),

$$\mathbf{P}=\begin{bmatrix}(e^{\sigma}+\frac14e^{-\sigma}) & -i(e^{\sigma}-\frac14e^{-\sigma})\\ i(e^{\sigma}-\frac14e^{-\sigma}) & (e^{\sigma}+\frac14e^{-\sigma})\end{bmatrix}\;,$$

satisfying the general requirements (see Ref. [8], p.107 or Ref. [5], p.143):

$$\begin{aligned}&P_{12}=-P_{12}^*=-P_{21}=P_{21}^*\;,\\ &P_{11}=P_{22}^*\quad\text{and}\quad\det[\mathbf{P}]=1\;.\end{aligned}$$

Note that neglecting the $e^{-\sigma}$ terms or dropping the e^{σ} terms [1)] would produce the disastrous result $\det[\mathbf{P}]=0$! Thus, we shall drop neither of the two terms, learning in the process that both the decaying and the boosting through the barrier are required for a consistent description of tunneling!

Solving for (A',B) in terms of (A,B'), we have Thus,

$$\begin{aligned}A'&=\frac{1}{e^{\sigma}+\frac14e^{-\sigma}}A-i\frac{e^{\sigma}-\frac14e^{-\sigma}}{e^{\sigma}+\frac14e^{-\sigma}}B'\;,\\ B&=-i\frac{e^{\sigma}-\frac14e^{-\sigma}}{e^{\sigma}+\frac14e^{-\sigma}}A+\frac{1}{e^{\sigma}+\frac14e^{-\sigma}}B'\;,\end{aligned}\qquad\text{so}\quad\mathbf{S}=\begin{bmatrix}\frac{1}{e^{\sigma}+\frac14e^{-\sigma}} & -i\frac{e^{\sigma}-\frac14e^{-\sigma}}{e^{\sigma}+\frac14e^{-\sigma}}\\ -i\frac{e^{\sigma}-\frac14e^{-\sigma}}{e^{\sigma}+\frac14e^{-\sigma}} & \frac{1}{e^{\sigma}+\frac14e^{-\sigma}}\end{bmatrix}\;.$$

Indeed, $\mathbf{S}^{\dagger}=\mathbf{S}^{-1}$ and $\det[\mathbf{S}]=1$.

Now consider the situation in which a right-moving wave (amplitude A) approaches the potential from the left (in region I). Part of it will reflect (amplitude B) as a left-mover in region I, and part of it (amplitude A') is transmitted as a right-mover into region III. Note that there is no in-coming (left-mover) wave in region III, whence we set $B'=0$.

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1) The substitution $e^{\sigma}\pm\frac14e^{-\sigma}\to\pm\frac14e^{-\sigma}$ is done in some books, when attempting to describe an incomming wave from left, with the amplitude A, being reflected into the left-mover in region I, with amplitude B, and partially tunneling into the right mover in region III, whence the boost by e^{σ} is dropped to retain only the desirable $e^{-\sigma}$-damping.

To determine the transmittivity and and reflectivity of the barrier, it is convenient to obtain and intermediate result: starting with either of the two WKB partial waves,

$$
\begin{aligned}
j &= \frac{\hbar}{2mi}\big[\psi^*\frac{\mathrm{d}}{\mathrm{d}x}\psi - \psi\frac{\mathrm{d}}{\mathrm{d}x}\psi^*\big]~, \\
&= \frac{\hbar|N|^2}{2mi}\Big[\frac{e^{\pm iK(x)}}{\sqrt{k}(x)}\frac{\mathrm{d}}{\mathrm{d}x}\frac{e^{\mp iK(x)}}{\sqrt{k}(x)} - \frac{e^{\mp iK(x)}}{\sqrt{k}(x)}\frac{\mathrm{d}}{\mathrm{d}x}\frac{e^{\pm iK(x)}}{\sqrt{k}(x)}\Big]~, \\
&= \frac{\hbar|N|^2}{2mi}\Big[\frac{e^{\pm iK(x)}}{\sqrt{k}(x)}\Big(\frac{\mp ik(x)e^{\mp iK(x)}}{\sqrt{k}(x)} - \tfrac{1}{2}\frac{k'(x)e^{\mp iK(x)}}{\sqrt{k^3(x)}}\Big) \\
&\qquad - \frac{e^{\mp iK(x)}}{\sqrt{k}(x)}\Big(\frac{\pm ik(x)e^{\pm iK(x)}}{\sqrt{k}(x)} - \tfrac{1}{2}\frac{k'(x)e^{\pm iK(x)}}{\sqrt{k^3(x)}}\Big)\Big]~, \\
&= \frac{\hbar|N|^2}{2mi}\Big[\big(\pm i - \frac{k'(x)}{2k^2(x)}\big) - \big(\mp i - \frac{k'(x)}{2k^2(x)}\big)\Big] = \pm\frac{\hbar|N|^2}{m}~,
\end{aligned}
\tag{1.5}
$$

where N is the amplitude of the partial wave, $K(x) \stackrel{\text{def}}{=} \int_{x_*}^{x} \mathrm{d}\xi~k(\xi)$, so $K'(x) = k(x)$ and the sign of the current indicates right/left motion. Note that the WKB amplitudes, here N and A, B, C, D in Eqs. (1.3), have the dimensions of (length)$^{-1}$.

Using Eqs. (1.4) and (1.5), we find (see also Ref. [9], p.67):

$$
T = \left|\frac{A'}{A}\right|^2 = |S_{11}|^2 = \frac{1}{(e^\sigma + \frac{1}{4}e^{-\sigma})^2}~,
$$

and similarly,

$$
R = \left|\frac{B}{A}\right|^2 = |S_{21}|^2 = \Big(\frac{e^\sigma - \frac{1}{4}e^{-\sigma}}{e^\sigma + \frac{1}{4}e^{-\sigma}}\Big)^2~.
$$

It is easy to verify that $T + R = 1$, as required.

It is also of practical value to expand T in powers of $e^{-2\sigma}$:

$$
\begin{aligned}
T &= \frac{1}{(e^\sigma + \frac{1}{4}e^{-\sigma})^2} = e^{-2\sigma}(1 + \tfrac{1}{4}e^{-2\sigma})^{-2}~, \\
&= e^{-2\sigma}\Big[1 + \sum_{n=1}^{\infty}\binom{-2}{n}\frac{e^{-2n\sigma}}{4^n}\Big] = e^{-2\sigma}\Big[1 + \sum_{n=1}^{\infty}(-1)^n\frac{n{+}1}{4^n}e^{-2n\sigma}\Big]~, \\
&= e^{-2\sigma}\Big[1 - \tfrac{1}{2}e^{-2\sigma} + \tfrac{3}{16}e^{-4\sigma} - \tfrac{1}{16}e^{-6\sigma} + \dots\Big]
\end{aligned}
\tag{1.6}
$$

where $\binom{-2}{n}$ is most easily evaluated using that [2]:

$$
\binom{N}{n} = \frac{N!}{(N{-}n)!n!} = \frac{N[N{-}1]\cdots[N{-}(n{-}1)](N{-}n)!}{(N{-}n)!n!} = \underbrace{\frac{N}{1}\cdot\frac{N{-}1}{2}\cdots\frac{N{-}n{+}1}{n}}_{n\text{ terms}}~.
$$

[2] Note: without the peculiar $\frac{1}{2}$ in the matching conditions, there would be no $\frac{1}{4}$ in Eq. (1.6), T would become $\mathrm{sech}^2(\sigma)$ and would fail to converge as a power series in $e^{-2\sigma}$.

Thus, for $e^{-2\sigma} \ll 1$, $T \approx e^{-2\sigma}$ is indeed a very good approximation.

2. Variational Method: Simple Power Potentials

Consider a particle moving in one dimension, under the influence of the potential $\lambda|x|^\gamma$. Its Hamiltonian is

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \lambda|x|^\gamma \ , \qquad \gamma > 0 \ . \tag{2.1}$$

For $\gamma \leq 0$, $\lim_{x\to\infty} V(x) \to 0$, in which case we know that the wave-function must decay exponentially at $x \to \infty$; hence the restriction to $\gamma > 0$. Steeper potentials (larger and larger γ) will induce an increasingly steeper exponential decay. We therefore look for the lowest energy wave-function of the general form $|0\rangle = C\exp[-\frac{1}{2}(\beta|x|)^\alpha]$. Since the normalization constant, C, is a fixed function of α, β, we must choose the parameters α, β so as to minimize $E = \langle 0|\hat{H}|0\rangle$.

2.1. Normalization

Requiring that $\langle 0|\mathbb{1}|0\rangle = 1$, we obtain, using the Gamma functions integral (see appendix),

$$|C|^{-2} = \int_{-\infty}^{+\infty}\mathrm{d}x\ e^{-(\beta|x|)^\alpha} = 2\int_0^{+\infty}\mathrm{d}x\ e^{-(\beta x)^\alpha} = \frac{2\Gamma(\frac{1}{\alpha})}{\alpha\,\beta} \ , \tag{2.2}$$

and so

$$C = \sqrt{\frac{\alpha\,\beta}{2\Gamma(\frac{1}{\alpha})}} \ . \tag{2.3}$$

We will also need

$$\begin{aligned} \frac{\mathrm{d}^2}{\mathrm{d}x^2}\, e^{-\frac{1}{2}(\beta x)^\alpha} &= \Big[\big(-\tfrac{\alpha}{2}\beta^\alpha x^{\alpha-1}\big)^2 - \tfrac{\alpha(\alpha-1)}{2}\beta^\alpha x^{\alpha-2}\Big]e^{-\frac{1}{2}(\beta x)^\alpha} \\ &= \Big[\tfrac{\alpha^2}{4}\beta^{2\alpha}x^{2\alpha-2} - \tfrac{\alpha(\alpha-1)}{2}\beta^\alpha x^{\alpha-2}\Big]e^{-\frac{1}{2}(\beta x)^\alpha} \ . \end{aligned} \tag{2.4}$$

2.2. Energy

Now is is easy to evaluate

$$E = C^2\int_{-\infty}^{+\infty}\mathrm{d}x\ e^{-\frac{1}{2}(\beta|x|)^\alpha}\Big[-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \lambda|x|^\gamma\Big]e^{-\frac{1}{2}(\beta|x|)^\alpha} \ , \tag{2.5a}$$

$$= \frac{\alpha\,\beta}{\Gamma(\frac{1}{\alpha})}\int_0^{+\infty}\mathrm{d}x\ e^{-\frac{1}{2}(\beta x)^\alpha}\Big[-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \lambda x^\gamma\Big]e^{-\frac{1}{2}(\beta x)^\alpha} \ , \tag{2.5b}$$

$$= \frac{\alpha\,\beta}{\Gamma(\frac{1}{\alpha})}\int_0^{+\infty}\mathrm{d}x\ e^{-(\beta x)^\alpha}\Big[-\frac{\hbar^2}{2m}\Big(\tfrac{\alpha^2}{4}\beta^{2\alpha}x^{2\alpha-2} - \tfrac{\alpha(\alpha-1)}{2}\beta^\alpha x^{\alpha-2}\Big) + \lambda x^\gamma\Big] \ , \tag{2.5c}$$

$$= \frac{\alpha\,\beta}{\Gamma(\frac{1}{\alpha})}\Big[-\frac{\hbar^2}{2m}\Big(\tfrac{\alpha^2}{4}\beta^{2\alpha}\frac{\Gamma(\frac{2\alpha-1}{\alpha})}{\alpha\,\beta^{2\alpha-1}} - \tfrac{\alpha(\alpha-1)}{2}\beta^{\alpha}\frac{\Gamma(\frac{\alpha-1}{\alpha})}{\alpha\,\beta^{\alpha-1}}\Big) + \lambda\frac{\Gamma(\frac{\gamma+1}{\alpha})}{\alpha\,\beta^{\gamma+1}}\Big]\ , \tag{2.5d}$$

$$= \frac{\alpha\,\beta}{\Gamma(\frac{1}{\alpha})}\Big[\frac{\hbar^2}{2m}\Big(\tfrac{(\alpha-1)\beta}{2}\Gamma(1-\tfrac{1}{\alpha}) - \tfrac{\alpha\beta}{4}\Gamma(2-\tfrac{1}{\alpha})\Big) + \lambda\frac{\Gamma(\frac{\gamma+1}{\alpha})}{\alpha\,\beta^{\gamma+1}}\Big]\ , \tag{2.5e}$$

$$= \frac{\hbar^2}{2m}\Big(\tfrac{\alpha(\alpha-1)}{2}\frac{\Gamma(1-\frac{1}{\alpha})}{\Gamma(\frac{1}{\alpha})} - \tfrac{\alpha^2}{4}\frac{\Gamma(2-\frac{1}{\alpha})}{\Gamma(\frac{1}{\alpha})}\Big)\beta^2 \ +\ \lambda\frac{\Gamma(\frac{\gamma+1}{\alpha})}{\Gamma(\frac{1}{\alpha})}\beta^{-\gamma}\ . \tag{2.5f}$$

2.3. Exponent

Because of the highly transcendental dependence on α, here we minimize this expression for energy only with respect to β. We will select α based on the asymptotic behavior of the wave-functions.

For very large x, the first term in Eq. (2.4) is always bigger, since α is non-negative (for the wave-function $|0\rangle = C\exp[-\frac{1}{2}(\beta|x|)^{\alpha}]$ to vanish at $x\to\infty$). Thus, the Schrödinger equation becomes

$$\Big[-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \lambda|x|^{\gamma}\Big]\,|0\rangle\ = E\,|0\rangle\ , \tag{2.6a}$$

$$\Big[-\frac{\hbar^2}{2m}\Big(\tfrac{\alpha^2}{4}\beta^{2\alpha}x^{2\alpha-2} - \tfrac{\alpha(\alpha-1)}{2}\beta^{\alpha}x^{\alpha-2}\Big) + \Big(\lambda|x|^{\gamma} - E\Big)\Big]\,|0\rangle\ = 0\ , \tag{2.6b}$$

$$\Big[-\frac{\hbar^2}{2m}\Big(\tfrac{\alpha^2}{4}\beta^{2\alpha}x^{2\alpha-2}\Big) + \lambda|x|^{\gamma}\Big]\,|0\rangle\ \approx 0\ . \tag{2.6c}$$

For the last line, we neglected E as compared to $\lambda|x|^{\gamma}$, and $x^{\alpha-2}$ as compared to $x^{2\alpha-2}$. For Eq. (2.6c) to hold, we must have $2\alpha-2=\gamma$, and so $\alpha=\frac{1}{2}\gamma+1$. Indeed, $\gamma=0$ corresponds to (asymptotically) constant potentials, for which $|0\rangle\sim e^{-\kappa x}$, and for the linear harmonic oscillator, $\gamma=2$ and so $|0\rangle\sim e^{-\sigma x^2}$; where $\kappa,\sigma>0$ are suitable constants.

2.4. Damping

We are now ready to minimize (2.5f) with respect to β: we see that $E = A\beta^2 + B\beta^{-\gamma}$, where $A=\frac{\hbar^2}{2m}\Big(\frac{\alpha(\alpha-1)}{2}\frac{\Gamma(1-\frac{1}{\alpha})}{\Gamma(\frac{1}{\alpha})} - \frac{\alpha^2}{4}\frac{\Gamma(2-\frac{1}{\alpha})}{\Gamma(\frac{1}{\alpha})}\Big)$ and $B=\lambda\frac{\Gamma(\frac{\gamma+1}{\alpha})}{\Gamma(\frac{1}{\alpha})}$ are two constants. Easily:

$$\frac{\partial E}{\partial\beta} = \Big(2A - \gamma B\beta^{-\gamma}\Big)\beta\ . \tag{2.7}$$

The two extrema are $\beta=0$ and $\beta=\sqrt[\gamma]{\frac{\gamma B}{2A}}$. The Reader will easily verify that this agrees with the results for the familiar cases $\gamma=0,2$.

Appendix A. Some Useful Integrals

The following formulae are results of fairly standard integration techniques.

A.1. Symmetric limits

Any integral with finite definite limits can be brought into the form with symmetric limits:

$$\int_a^b \mathrm{d}x\ f(x) \;=\; \int_{-L}^{+L} \mathrm{d}\xi\ f(\xi)\ ,$$

where $L = \frac{1}{2}(b{-}a)$ and $\xi = x - \frac{1}{2}(b{+}a)$. Thereafter, we write

$$\begin{aligned}\int_{-L}^{+L} \mathrm{d}\xi\ f(\xi) &= \int_{-L}^{0} \mathrm{d}\xi\ f(\xi) + \int_{0}^{+L} \mathrm{d}\xi\ f(\xi) = \int_{+L}^{0} \mathrm{d}(-\xi)\ f(-\xi) + \int_0^L \mathrm{d}(\xi)\ f(\xi)\ ,\\ &= -\int_0^{+L} \mathrm{d}(-\xi)\ f(-\xi) + \int_0^L \mathrm{d}(\xi)\ f(\xi) = \int_0^{+L} \mathrm{d}\xi\ \big[f(\xi) + f(-\xi)\big]\ .\end{aligned}$$

Clearly now, if $f(-\xi) = -f(\xi)$, the integral vanishes; on the other hand, if $f(-\xi) = +f(\xi)$, the two terms add up to $2f(\xi)$.

A.2. Gamma function evaluations

Any integral of the type $\int_0^L \mathrm{d}x\ e^{-\alpha x^\beta} x^\kappa$, with $\Re e(\beta) > 0$, can be evaluated using the incomplete (complete) Gamma function, the definitions of which are

$$\gamma(\nu;\mu) \stackrel{\text{def}}{=} \int_0^\mu \mathrm{d}t\ e^{-t} t^{\nu-1}\ , \qquad \text{and} \qquad \Gamma(\nu) \stackrel{\text{def}}{=} \int_0^\infty \mathrm{d}t\ e^{-t} t^{\nu-1}\ .$$

To this end, one performs the substitution:

$$\begin{aligned}\int_0^L \mathrm{d}x\ e^{-\alpha x^\beta} x^\kappa &= \int_0^{\alpha L^\beta} \mathrm{d}t\ \Big(\frac{t}{\alpha}\Big)^{\frac{1}{\beta}} t^{-1}\ e^{-t} \Big(\frac{t}{\alpha}\Big)^{\frac{\kappa}{\beta}}\ , \qquad t \stackrel{\text{def}}{=} \alpha x^\beta\ ,\\ &= \alpha^{-\frac{\kappa+1}{\beta}} \int_0^{\alpha L^\beta} \mathrm{d}t\ e^{-t} t^{\frac{\kappa+1}{\beta}-1}\ ,\end{aligned}$$

This provides the "Gamma function evaluations":

$$\begin{aligned}\int_0^L \mathrm{d}x\ e^{-\alpha x^\beta} x^\kappa &= \alpha^{-\frac{\kappa+1}{\beta}} \gamma\big(\tfrac{\kappa+1}{\beta}; \alpha L^\beta\big)\ , \qquad \text{and}\\ \int_0^\infty \mathrm{d}x\ e^{-\alpha x^\beta} x^\kappa &= \alpha^{-\frac{\kappa+1}{\beta}} \Gamma\big(\tfrac{\kappa+1}{\beta}\big)\ .\end{aligned}$$

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