# Math 515
# Essential Perturbation Theory and Asymptotic Analysis
# Chapter 06

Steven M. Wise

swise1@.utk.edu
University of Tennessee

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# Chapter 06, Part 2 of 2
# The WKB Method

# The Quantum Harmonic Oscillator

## The Time-Dependent Schrödinger Equation

The time-dependent Schrödinger equation is given by

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V(x)\Psi, \quad x \in (-\infty, \infty), \tag{1}$$

where $\hbar$ is Planck's constant, $m$ is the mass of the particle, $V(x)$ is the potential energy of the particle, and $\Psi$ is a the wave function, which satisfies the normalization

$$\int_{-\infty}^{\infty} |\Psi(x,t)|^2 \, \mathrm{d}x = 1.$$

We assume that the following separation of variables is valid:

$$\Psi(x,t) = \psi(x)T(t).$$

It follows that

$$i\hbar \frac{1}{T}\frac{\mathrm{d}T}{\mathrm{d}t} = -\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + V.$$

## Separation

Since the function on the left is only a function of $t$ and the function on the right is only a function of $x$, there must be a separation constant $E$ such that

$$\mathrm{i}\hbar \frac{1}{T}\frac{\mathrm{d}T}{\mathrm{d}t} = E = -\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + V.$$

Though it is not clear at the moment, it will follow that $E > 0$. Furthermore,

$$T(t) = e^{-\mathrm{i}Et/\hbar},$$

and

$$-\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = \frac{2m}{\hbar^2}\left(E - V(x)\right)\psi.$$

The potential is that of a harmonic oscillator:

$$V(x) = \frac{1}{2}m\omega^2x^2,$$

where $\omega > 0$ is a constant. Thus, we seek a solution to the equation

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + \frac{1}{2}m\omega^2x^2\psi = E\psi.$$

## Boundary and Normalization Conditions

What are the boundary conditions? We require that

$$\lim_{x \to \pm\infty} \psi(x) = 0.$$

Furthermore, recalling the normalization of the wave function, we need to have

$$\begin{aligned} 1 &= \int_{-\infty}^{\infty} |\Psi(x,t)|^2 \, \mathrm{d}x \\ &= \int_{-\infty}^{\infty} e^{-\mathrm{i}Et/\hbar} \psi(x) \overline{\psi(x)} e^{\mathrm{i}Et/\hbar} \, \mathrm{d}x \\ &= \int_{-\infty}^{\infty} |\psi(x)|^2 \, \mathrm{d}x. \end{aligned}$$

In other words, $\psi$ should also be normalized.

## Solution via Hermite Polynomials

Thus, we have an eigenvalue problem. The solution to this problem is well-known and involves the Hermite polynomials. We find that eigenvalues are

$$E_n = \left(n + \frac{1}{2}\right) \hbar\omega, \quad n = 0, 1, 2, \ldots, \tag{2}$$

and the corresponding eigenfunctions are

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\xi) e^{-\xi^2/2}, \quad \xi = \sqrt{\frac{m\omega}{\hbar}} x, \tag{3}$$

where $H_n$ is the $n^{\text{th}}$ Hermite polynomial. See Table 1. These form an orthogonal family of polynomials and satisfy the orthonormality condition

$$\int_{-\infty}^{\infty} H_n(x) H_m(x) e^{-x^2} \, \mathrm{d}x = \sqrt{\pi} 2^n n! \delta_{m,n}, \qquad n, m \in \mathbb{N}_0 = \mathbb{N} \cup \{0\}. \tag{4}$$

| $n$ | $H_n(x)$ |
|---|---|
| 0 | $H_0(x) = 1$ |
| 1 | $H_1(x) = 2x$ |
| 2 | $H_2(x) = 4x^2 - 2$ |
| 3 | $H_3(x) = 8x^3 - 12x$ |
| 4 | $H_4(x) = 16x^4 - 48x^2 + 12$ |
| 5 | $H_5(x) = 32x^5 - 160x^3 + 120$ |
| 6 | $H_6(x) = 64x^6 - 480x^4 + 720x^2 - 120$ |
| 7 | $H_7(x) = 128x^7 - 1344x^5 + 3360x^3 - 1680x$ |
| 8 | $H_8(x) = 256x^8 - 3584x^6 + 13440x^4 - 13440x^2 + 1680$ |
| 9 | $H_9(x) = 512x^9 - 9216x^7 + 48384x^5 - 80640x^3 + 30240x$ |

Table: The first ten Hermite polynomials.

# Normalization of the Wave Function

As a consequence, we see clearly that

$$\begin{aligned}\int_{-\infty}^{\infty} |\psi_n(x)|^2 \, \mathrm{d}x &= \sqrt{\frac{m\omega}{\pi\hbar}} \int_{x=-\infty}^{x=\infty} H_n^2(\xi) e^{-\xi^2} \, \mathrm{d}x \\ &= \sqrt{\frac{\hbar}{m\omega}} \sqrt{\frac{m\omega}{\pi\hbar}} \frac{1}{2^n n!} \int_{\xi=-\infty}^{\xi=\infty} H_n^2(\xi) e^{-\xi^2} \, \mathrm{d}\xi \\ &= \sqrt{\frac{\hbar}{m\omega}} \sqrt{\frac{m\omega}{\pi\hbar}} \frac{1}{2^n n!} \sqrt{\pi} 2^n n! \\ &= 1,\end{aligned}$$

as desired. More generally, we have

$$\int_{-\infty}^{\infty} \psi_n(x)\psi_m(x) \, \mathrm{d}x = \delta_{m,n}.$$

# A Solution to the Time-Dependent Problem

Thus, the energy levels are quantized, and a general solution to the time-dependent Schrödinger equation may be given by the principle of superposition:

$$\Psi(x,t) = \sum_{k=0}^{\infty} c_k e^{-\mathrm{i}E_k t/\hbar} \psi_k(x). \tag{5}$$

The coefficients in the expansion are given by the initial data, as follows:

$$f(x) = \Psi(x, t=0) = \sum_{k=0}^{\infty} c_k \psi_k(x).$$

Using the orthonormality condition, we have

$$c_\ell = \int_{-\infty}^{\infty} f(x)\psi_\ell(x)\,\mathrm{d}x, \quad \ell = 0, 1, 2, \ldots.$$

These numbers, $c_\ell$, are sometimes called the Fourier coefficients.

## A Dimensionless Time-Independent Problem

The non-dimensional version of the problem is as follows:

$$\frac{\mathrm{d}^2 y}{\mathrm{d}\xi^2} = (\xi^2 - K)y(\xi), \quad \xi = \sqrt{\frac{m\omega}{\hbar}}x, \tag{6}$$

where

$$K = \frac{2E}{\hbar\omega} > 0.$$

This problem has two turning points. Setting $q(\xi) = \xi^2 - K$, we have turning points at

$$\xi = \pm\sqrt{K}.$$

In the next section, we will use the WKB method to approximate solutions to a generalized version of this problem.

# The Two-Turning-Point Eigenvalue Problem

# Two Turning Points

Consider the following Schrödinger equation

$$\varepsilon^2 y''(x) - q(x)y(x) = 0, \quad -\infty < x < \infty, \tag{7}$$

where $\varepsilon \in (0,1)$, with the "boundary" conditions

$$\lim_{x \searrow -\infty} y(x) = 0 \quad \text{and} \quad \lim_{x \nearrow \infty} y(x) = 0. \tag{8}$$

In this section, we address the case that $q$ changes sign twice on the domain $\Omega = (-\infty, \infty)$.

## Single-Well Potential

Specifically, we assume that

$$q(x) = V(x) - E,$$

where

1. $V(x) \geq 0$;
2. $V(x)$ has a global minimum at $x = c$;
3. $V(c) = 0$;
4. $V(r)$ is monotonically increasing as $r$ increases, where $r = |x - c|$;
5. $\lim_{x \nearrow \infty} V(x) = \infty$;
6. $\lim_{x \searrow -\infty} V(x) = \infty$.

For example, for any $p > 0$, the function

$$V(x) = |x - c|^p$$

satisfies the conditions. A potential $V$ that satisfies these conditions is called a **single-well potential energy**.

## Three Regions

It follows that, if $E > 0$, then there are exactly two points $x = \alpha = \alpha(E) < c$ and $x = \beta = \beta(E) > c$, such that

$$V(\alpha) = E \quad \text{and} \quad V(\beta) = E.$$

With respect to the value of $E$, the points $x = \alpha(E)$ and $x = \beta(E)$ represent the unique turning points for $q(x)$, and we have, precisely,

$$\begin{aligned} q(x) &> 0, \quad \forall\, x \in (-\infty, \alpha); \\ q(x) &< 0, \quad \forall\, x \in (\alpha, \beta); \\ q(x) &> 0, \quad \forall\, x \in (\beta, \infty). \end{aligned}$$

We can use our connection formulae to construct approximate solutions. In fact, all that is important for the determination of the eigenvalues, $E_k$, are the connection formulae in the interval $(\alpha, \beta)$, where the solution is expected to be oscillatory.

# The Connection Formulae Near $x = \beta$

Near $x = \beta$ the connection formulae satisfy

$$y(x;\varepsilon) \sim \begin{cases} \dfrac{2A_\beta}{\sqrt[4]{-q(x)}} \sin\left( \frac{1}{\varepsilon} \int_x^\beta \sqrt{-q(t)}\,\mathrm{d}t + \frac{\pi}{4} \right), & x \in (\alpha, \beta), \\ \dfrac{2\sqrt{\pi}A_\beta}{(\varepsilon a_\beta)^{1/6}} \mathrm{Ai}\left( \dfrac{a_\beta^{1/3}}{\varepsilon^{2/3}}(x-\beta) \right), & x \in \Omega_{I,\beta}, \\ \dfrac{A_\beta}{\sqrt[4]{q(x)}} \exp\left( -\frac{1}{\varepsilon} \int_\beta^x \sqrt{q(t)}\,\mathrm{d}t \right), & x \in (\beta, \infty), \end{cases} \tag{9}$$

where, as $x \to \beta$,

$$q(x) = a_\beta(x-\beta) + O((x-\beta)^2),$$

with $a_\beta > 0$. The constant $A_\beta$ is undetermined.

# The Connection Formulae Near $x = \alpha$

To find the connection formulae near $x = \alpha$, we need to be a bit more careful. We have

$$y(x;\varepsilon) \sim \begin{cases} \frac{A_\alpha}{\sqrt[4]{q(x)}} \exp\left(-\frac{1}{\varepsilon}\int_x^\alpha \sqrt{q(t)}\,\mathrm{d}t\right), & x \in (-\infty, \alpha), \\ \frac{2\sqrt{\pi}A_\alpha}{(\varepsilon a_\beta)^{1/6}} \mathrm{Ai}\left(\frac{a_\alpha^{1/3}}{\varepsilon^{2/3}}(\alpha - x)\right), & x \in \Omega_{I,\alpha}, \\ \frac{2A_\alpha}{\sqrt[4]{-q(x)}} \sin\left(\frac{1}{\varepsilon}\int_\alpha^x \sqrt{-q(t)}\,\mathrm{d}t + \frac{\pi}{4}\right), & x \in (\alpha, \beta), \end{cases} \tag{10}$$

where, as $x \to \alpha$,

$$q(x) = -a_\alpha(x-\alpha) + O((x-\alpha)^2),$$

with $a_\alpha > 0$.

# Joining Solutions in $(\alpha, \beta)$

In order to join these two sets of connection formulae, the respective solutions in the region $(\alpha, \beta)$ must agree precisely. In other words, we need to enforce

$$2A_\beta \frac{\sin\left(\frac{1}{\varepsilon}\int_x^\beta \sqrt{-q(t)}\,\mathrm{d}t + \frac{\pi}{4}\right)}{\sqrt[4]{-q(x)}} = 2A_\alpha \frac{\sin\left(\frac{1}{\varepsilon}\int_\alpha^x \sqrt{-q(t)}\,\mathrm{d}t + \frac{\pi}{4}\right)}{\sqrt[4]{-q(x)}}, \qquad (11)$$

for all $x \in (\alpha, \beta)$, which we call the *quantization condition*, because, as we will see, this forces a quantization of the energy levels.

## Some Definitions

Define

$$K_{\alpha,\beta} := \frac{1}{\varepsilon}\int_{\alpha}^{\beta}\sqrt{-q(t)}\,\mathrm{d}t + \frac{\pi}{2};$$

$$I_{\beta}(x) := \sin\left(\frac{1}{\varepsilon}\int_{x}^{\beta}\sqrt{-q(t)}\,\mathrm{d}t + \frac{\pi}{4}\right);$$

$$I_{\alpha}(x) := \sin\left(\frac{1}{\varepsilon}\int_{\alpha}^{x}\sqrt{-q(t)}\,\mathrm{d}t + \frac{\pi}{4}\right).$$

Then, the quantization condition (11) is equivalent to

$$A_{\beta}I_{\beta}(x) = A_{\alpha}I_{\alpha}(x), \tag{12}$$

for all $x \in (\alpha, \beta)$.

## Some Manipulation

Observe that

$$\begin{aligned}
l_\beta(x) &= \sin\left(\frac{1}{\varepsilon}\int_x^\beta \sqrt{-q(t)}\,\mathrm{d}t + \frac{\pi}{4}\right) \\
&= \sin\left(\frac{1}{\varepsilon}\int_\alpha^\beta \sqrt{-q(t)}\,\mathrm{d}t - \frac{1}{\varepsilon}\int_\alpha^x \sqrt{-q(t)}\,\mathrm{d}t + \frac{\pi}{4}\right) \\
&= -\sin\left(-\frac{1}{\varepsilon}\int_\alpha^\beta \sqrt{-q(t)}\,\mathrm{d}t + \frac{1}{\varepsilon}\int_\alpha^x \sqrt{-q(t)}\,\mathrm{d}t - \frac{\pi}{4}\right) \\
&= -\sin\left(\frac{1}{\varepsilon}\int_\alpha^x \sqrt{-q(t)}\,\mathrm{d}t + \frac{\pi}{4} - \frac{1}{\varepsilon}\int_\alpha^\beta \sqrt{-q(t)}\,\mathrm{d}t - \frac{\pi}{2}\right) \\
&= -\sin\left(\frac{1}{\varepsilon}\int_\alpha^x \sqrt{-q(t)}\,\mathrm{d}t + \frac{\pi}{4}\right)\cos(K_{\alpha,\beta}) \\
&\quad + \cos\left(\frac{1}{\varepsilon}\int_\alpha^x \sqrt{-q(t)}\,\mathrm{d}t + \frac{\pi}{4}\right)\sin(K_{\alpha,\beta}) \\
&= l_\alpha(x)\cos(K_{\alpha,\beta}) + \cos\left(\frac{1}{\varepsilon}\int_\alpha^x \sqrt{-q(t)}\,\mathrm{d}t + \frac{\pi}{4}\right)\sin(K_{\alpha,\beta}).
\end{aligned}$$

## Energy Quantization

To ensure that (12) holds, we require that

$$\sin(K_{\alpha,\beta}) = 0.$$

This implies that

$$K_{\alpha,\beta} = \frac{1}{\varepsilon}\int_{\alpha}^{\beta}\sqrt{-q(t)}\,\mathrm{d}t + \frac{\pi}{2} = k\pi,$$

where $k$ is an integer. Since $K_{\alpha,\beta} > 0$, $k$ must be a positive integer. Thus,

$$\frac{1}{\varepsilon}\int_{\alpha}^{\beta}\sqrt{-q(t)}\,\mathrm{d}t = \left(k - \frac{1}{2}\right)\pi, \quad k = 1, 2, \ldots,$$

or, equivalently,

$$\frac{1}{\varepsilon}\int_{\alpha}^{\beta}\sqrt{E_k - V(x)}\,\mathrm{d}t = \left(k - \frac{1}{2}\right)\pi, \quad k = 1, 2, \ldots.$$

# The First and Second Quantization Rules

The last equation,

$$\frac{1}{\varepsilon}\int_{\alpha}^{\beta}\sqrt{E_k - V(x)}\,\mathrm{d}t = \left(k - \frac{1}{2}\right)\pi, \quad k = 1, 2, \ldots, \tag{13}$$

indicates that the energy levels must be quantized! This last relation, Equation (13), is called the *first quantization rule*.

To finish up, we have

$$I_\beta = I_\alpha \cos(k\pi) = I_\alpha (-1)^k, \quad k \in \mathbb{N},$$

and, therefore

$$A_\beta I_\beta = A_\alpha I_\alpha,$$

iff

$$A_\beta (-1)^k = A_\alpha, \tag{14}$$

which we refer to as the *second quantization rule*.

## WKB Validity

Finally, we point out that our WKB approximations herein are valid, provided either

1. $\varepsilon \searrow 0$, that is, $\varepsilon$ is small, and/or,
2. $k \nearrow \infty$, that is, the energy levels are high.

## Example

In this example, we examine a non-dimensional version of the quantum harmonic oscillator. Suppose that $V(x) = x^2$ and $\varepsilon = 1$. Then, in this case,

$$\alpha = -\sqrt{E_k} \quad \text{and} \quad \beta = \sqrt{E_k},$$

and

$$\frac{1}{\varepsilon}\int_{\alpha}^{\beta} \sqrt{E_k - V(x)}\,\mathrm{d}t = \sqrt{E_k}\int_{-\sqrt{E_k}}^{\sqrt{E_k}} \sqrt{1 - \left(\frac{x}{\sqrt{E_k}}\right)^2}\,\mathrm{d}t$$
$$= E_k \frac{\pi}{2}.$$

The quantization rule (13) implies that

$$E_k = 2\left(k - \frac{1}{2}\right), \quad k = 1, 2, \ldots .$$

## Example (Cont.)

In this example, (7) can be written as

$$-y''(x) + x^2 y(x) = E y(x), \tag{15}$$

and the boundary conditions are

$$\lim_{x \searrow -\infty} y(x) = 0 \quad \text{and} \quad \lim_{x \nearrow \infty} y(x) = 0. \tag{16}$$

The exact eigenvalues are

$$E_k = 2\left(k + \frac{1}{2}\right), \quad k = 0, 1, 2, \ldots,$$

and the associated eigenfunctions are

$$y_k(x) = \frac{1}{\pi^{1/4}} \frac{1}{\sqrt{2^k k!}} H_k(x) e^{-x^2/2}, \quad k = 0, 1, 2, \ldots,$$

using the normalization

$$\int_{-\infty}^{\infty} |y_k(x)|^2 \, \mathrm{d}x = 1.$$

### Example (Cont.)

So, we observe that, for this example, our WBK approximation, yields the exact eigenvalues.