Nondegenerate Time Independent Perturbation Theory

Reference:
Griffiths 7.1

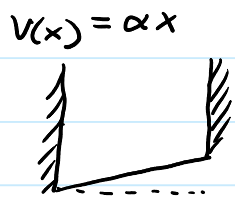
When trying to solve the Schrödinger Equation in QM, we find that there are only a few special potentials $V(\vec{r})$ where you can solve for $\psi(\vec{r})$ exactly. The ones you <u>can</u> solve exactly (at least the ones I know) are:

- Infinite Well (rectangular, spherical, cylindrical)
- Harmonic Oscillator
- Free particle
- δ-function potential
- Hydrogen-like atom (Coulomb potential).

Unsurprisingly, these are <u>all</u> the systems we've studied so far in this course. I hate to be the bearer of bad news, but we're basically reaching the limit of what can be done exactly. Current physics research relies much more on approximate solutions than on exact solutions, so its time that we turn to this approach.

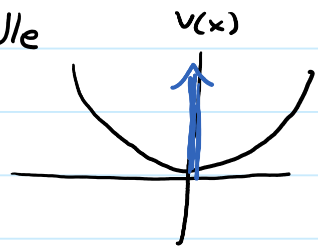
Let's focus now on a potential which is <u>close</u> to one of the systems we've discussed before, but with a <u>small</u> difference.

<u>Examples:</u>



① An infinite square well with a slight slope

② A harmonic oscillator with a δ-function in the middle



③ A hydrogen atom in a small electric or magnetic field.

⋮

etc... Basically we're interested in slight variations or perturbations on what we've studied before.

Nondegenerate Time Independent Perturbation Theory

Perturbation theory is a systematic way to tackle problems of this type here's the main idea:

Suppose you're trying to solve the time independent Schrödinger equation $\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle$, and the Hamiltonian can be written as

$$\hat{H} = \hat{H}^0 + \hat{H}^1$$

$\hat{H}^1$ is the perturbation, or deviation from what we already know.

$\hat{H}^0$ is the "unperturbed Hamiltonian". This is a Hamiltonian where you know the solutions already. We call these solutions ψ_n^0, and their energies are E_n^0. In other words

$$\hat{H}^0|\psi_n^0\rangle = E_n^0|\psi_n^0\rangle \quad \text{and we already know } |\psi_n^0\rangle, E_n^0$$

The idea is to assume the perturbation is <u>small</u> in some sense, so that we just need to find corrections to the energies and wave functions. For this purpose, let me introduce a "bookkeeping parameter", λ so that

$$\hat{H} = \hat{H}^0 + \lambda\hat{H}^1 \qquad \text{if } \lambda \to 0 \text{ I have no perturbation.}$$

We now assume ψ_n and E_n can be written as a power series in λ

that's $\psi^{(2)}$, not ψ-squared.

$$|\psi_n\rangle = |\psi_n^0\rangle + \lambda|\psi_n^1\rangle + \lambda^2|\psi_n^2\rangle + \ldots$$
$$E_n = E_n^0 + \lambda E_n^1 + \lambda E_n^2 + \ldots$$

Plug into the Schrödinger equation:

$$(\hat{H}^0 + \lambda\hat{H}^1)(|\psi_n^0\rangle + \lambda|\psi_n^1\rangle + \lambda^2|\psi_n^2\rangle + \ldots)$$
$$= (E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \ldots)(|\psi_n^0\rangle + \lambda|\psi_n^1\rangle + \lambda^2|\psi_n^2\rangle + \ldots)$$

Expand both sides and collect powers of λ:

$$\cancel{\hat{H}^0|\psi_n^0\rangle} + \lambda\left[\hat{H}^0|\psi_n^1\rangle + \hat{H}^1|\psi_n^0\rangle\right] + \lambda^2\left[\hat{H}^0|\psi^2\rangle + \hat{H}^1|\psi^1\rangle\right]$$
$$= \cancel{E_n^0|\psi_n^0\rangle} + \lambda\left[E_n^0|\psi_n^1\rangle + E_n^1|\psi_n^0\rangle\right] + \lambda^2\left[E_n^0|\psi_n^2\rangle + E_n^1|\psi_n^1\rangle + E_n^2|\psi_n^0\rangle\right],$$

By assumption, $\hat{H}^0\psi_n^0 = E_n^0\psi_n^0$.

Now the terms proportional to λ are first order in the perturbation.
" " " λ^2 are second order " " "

Since we assume the perturbation is a small correction, the terms of order λ^2 will be $(\text{small})^2$ and so lets ignore these for the time being. This gives:

λ is just a bookkeeping device anyway...

$$\cancel{\lambda}\left[\hat{H}^0|\psi_n^1\rangle + \hat{H}^1|\psi_n^0\rangle\right] = \cancel{\lambda}\left[E_n^0|\psi_n^1\rangle + E_n^1|\psi_n^0\rangle\right]$$

Now, multiply on the left by $\langle\psi_m^0|$

$$\underbrace{\langle\psi_m^0|\hat{H}^0|\psi_n^1\rangle} + \langle\psi_m^0|\hat{H}^1|\psi_n^0\rangle = E_n^0\langle\psi_m^0|\psi_n^1\rangle + E_n^1\underbrace{\langle\psi_m^0|\psi_n^0\rangle}_{\text{Orthonormal, } \delta_{nm}}$$

Claim: $\langle\psi_m^0|\hat{H}^0|\psi_n^1\rangle = E_m^0\langle\psi_m^0|\psi_n^1\rangle$

proof:

$$\hat{H}^0|\psi_m^0\rangle = E_m^0|\psi_m^0\rangle$$
$$\langle\psi_m^0|(\hat{H}^0)^\dagger = \langle\psi_m^0|E_m^0 \qquad \text{Definition of Adjoint}$$
$$\langle\psi_m^0|\hat{H}^0 = \langle\psi_m^0|E_m^0 \qquad \hat{H}^0 \text{ is Hermitian } (\hat{H}^0)^\dagger = \hat{H}^0$$
$$\langle\psi_m^0|\hat{H}^0|\psi_n^1\rangle = E_m^0\langle\psi_m^0|\psi_n^1\rangle \qquad \text{multiply on right by } |\psi_n^1\rangle$$

So, we have, then

$$\langle\psi_m^0|\hat{H}^1|\psi_n^0\rangle = (E_n^0 - E_m^0)\langle\psi_m^0|\psi_n^1\rangle + E_n^1\delta_{n,m}$$

So, we have, then

$$(*) \quad \langle \psi_m^0 | \hat{H}' | \psi_n^0 \rangle = (E_n^0 - E_m^0) \langle \psi_m^0 | \psi_n^1 \rangle + E_n^1 \delta_{n,m}$$

Now we focus on 2 cases:

1. $n = m$
2. $m \neq m$

Correction to energies: $(n = m)$

For $n = m$, the equation $(*)$ becomes:

$$\boxed{E_n^1 = \langle \psi_n^0 | \hat{H}' | \psi_n^0 \rangle}$$

The corrections to the energy E_n^1 are the expectation value of $\hat{H}'$, the perturbed Hamiltonian, in the unperturbed state ψ_n^0.

Put another way, E_n^1 = the diagonal matrix elements of $\hat{H}'$ in the unperturbed energy basis.

PollQ: In the unperturbed energy basis, suppose $\hat{H} = \varepsilon \begin{pmatrix} 1-\alpha & \alpha \\ \alpha & 2+2\alpha \end{pmatrix}$

Where α is a small parameter. What is the ground state energy to first order in α? No determinants allowed!

A.) $\varepsilon(1+\alpha)$ C.) $\varepsilon(2+2\alpha)$

B.) $\varepsilon(1-\alpha)$ D.) $\varepsilon(2-2\alpha)$

Note: If you calculate the eigenvalues exactly, you get

$$E = \frac{\varepsilon}{2}\left[3+\alpha \pm \sqrt{1+6\alpha+13\alpha^2}\,\right]$$

you can check, if you do a Taylor expansion around $\alpha = 0$, that you get the same answer to leading order in α.

Corrections to the states $|\psi_n\rangle$ – case 2, $n \neq m$

Now, return to equation (*). For $n \neq m$ we have:

$$(*) \quad \langle \psi_m^0 | \hat{H}' | \psi_n^0 \rangle = (E_n^0 - E_m^0)\langle \psi_m^0 | \psi_n^1 \rangle + \cancel{E_n^1 \delta_{n,m}}^{\,0}$$

$$\langle \psi_m^0 | \psi_n^1 \rangle = \frac{\langle \psi_m^0 | \hat{H}' | \psi_n^0 \rangle}{E_n^0 - E_m^0}$$

Let's see what this equation is good for. We're interested in the state vector correction $|\psi_n^1\rangle$. Just as for any state, we can express this as a combination of the unperturbed energy eigenstates. This is possible since $\{|\psi_n^0\rangle\}$ is complete (they span the space).

So, $|\psi_n^1\rangle = \sum_k c_{nk} |\psi_k^0\rangle$ — if we know the coefficients c_{mn}, we know $|\psi_n^1\rangle$!

now, multiply by $\langle \psi_m^0 |$

$$\langle \psi_m^0 | \psi_n^1 \rangle = \sum_k c_{nk} \langle \psi_m^0 | \psi_k^0 \rangle = \sum_k c_{nk} \cdot \delta_{mk} = c_{mn}$$

So, looking back up above, we see that

$$c_{mn} = \frac{\langle \psi_m^0 | \hat{H}' | \psi_n^0 \rangle}{E_n^0 - E_m^0}$$

, which allows us to determine $|\psi_n^1\rangle$.

In summary:

$$\boxed{|\psi_n^1\rangle = \sum_{m\neq n} \frac{\langle \psi_m^0|\hat{H}'|\psi_n^0\rangle}{E_n^0 - E_m^0} \cdot |\psi_m^0\rangle}$$

In words: the non-diagonal matrix elements of $\hat{H}'$ in the old, unperturbed energy basis allow us to determine the corrections to the eigenfunctions.

Subtle point: We only determined the coefficients c_{mn} when $m \neq n$. Shouldn't there be a term $c_{nn}|\psi_n^0\rangle$ on the right?

Claim: This term is zero.

Proof: $|\psi_n^1\rangle = \sum_m c_{mn}|\psi_m^0\rangle$ since $\{|\psi_m^0\rangle\}$ are complete.

$$|\psi_n^1\rangle = \sum_{m\neq n} c_{mn}|\psi_m^0\rangle + c_{nn}|\psi_n^0\rangle$$

I can choose, without loss of generality, to have c_{nn} real. This is because I can always multiply the state $|\psi\rangle$ by $e^{i\phi}$ and no physics changes since this does not affect any probability which involves $|\langle\chi|\psi\rangle|^2$.

Now, require $|\psi_n\rangle = |\psi_n^0\rangle + |\psi_n^1\rangle$ be normalized to first order in the perturbation

$$1 = \langle\psi_n|\psi_n\rangle = \left(\langle\psi_n^0| + \langle\psi_n^1|\right)\left(|\psi_n^0\rangle + |\psi_n^1\rangle\right)$$

$$= \langle\psi_n^0|\psi_n^0\rangle + \langle\psi_n^1|\psi_n^0\rangle + \langle\psi_n^0|\psi_n^1\rangle + 2^{\text{nd}}\text{ order terms}$$

$$\cancel{1} = \cancel{1} + \langle\psi_n^1|\psi_n^0\rangle + \langle\psi_n^0|\psi_n^1\rangle$$

(unperturbed states are normalized)

Now: $\langle \psi_n^0 | \psi_n^1 \rangle = \sum_{m \neq n} c_{mn} \underbrace{\cancel{\langle \psi_n^0 | \psi_m^0 \rangle}}_{\text{(orthogonal)}}^{0} + c_{nn} \underbrace{\cancel{\langle \psi_n^0 | \psi_n^0 \rangle}}_{\text{normalized.}}^{1}$

$\therefore \quad 0 = c_{nn} + c_{nn}^*$ since c_{nn} is real, by choice, it must be zero.

$0 = 2c_{nn}$

In summary:

$$|\psi_n^1\rangle = \sum_{m \neq n} \frac{\langle \psi_m^0 | \hat{H}' | \psi_n^0 \rangle}{E_n^0 - E_m^0} \cdot |\psi_m^0\rangle$$

PollQ: In the unperturbed energy basis, suppose $\hat{H} = \varepsilon \begin{pmatrix} 1-\alpha & \alpha \\ \alpha & 2+2\alpha \end{pmatrix}$

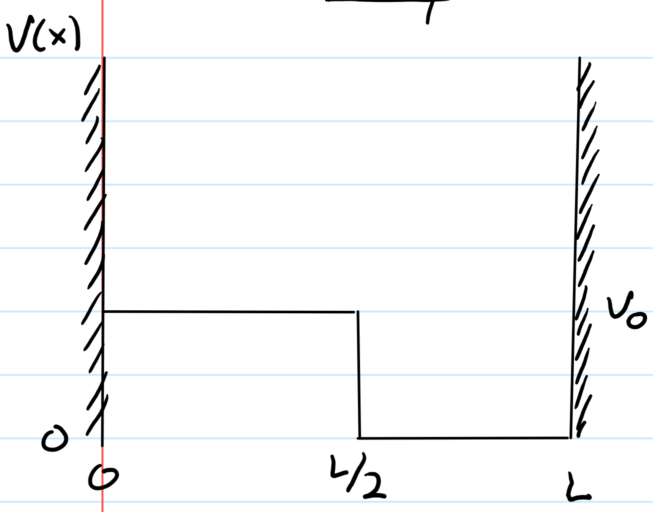
Where α is a small parameter. What is the ground state $|\psi_1\rangle$ to first order in α? No determinants allowed!

A.) $\begin{pmatrix} \alpha \\ 1 \end{pmatrix}$ C.) $\begin{pmatrix} 1 \\ 2\alpha \end{pmatrix}$

B.) $\begin{pmatrix} 1 \\ -\alpha \end{pmatrix}$ D.) $\begin{pmatrix} 2\alpha \\ 1 \end{pmatrix}$

Griffiths Example 7.1

An infinite square well has an uneven bottom as shown. Treat V_0 as a perturbation, and find the ground state energy and wave function to lowest order in V_0.



$$\hat{H} = \frac{\hat{p}^2}{2m} + V_0 \qquad 0 < x < \frac{L}{2}$$

$$\hat{H} = \hat{p}^2/2m \qquad \frac{L}{2} < x < L$$

$\hat{H}'$

Energy: $E_1^0 = \dfrac{\pi^2\hbar^2}{2mL^2}$ $\qquad E_1^1 = \langle \psi_1^0 | \hat{H}' | \psi_1^0 \rangle$

$$E_1^1 = \int_0^L \psi_1^0(x)^* \cdot V_0 \cdot \psi_1^0(x)\, dx$$

$$E_1^1 = V_0 \cdot \int_0^{L/2} \frac{2}{L} \cdot \sin^2\left(\frac{\pi x}{L}\right) dx$$

Let $u = \dfrac{\pi x}{L}$

$du = \dfrac{\pi dx}{L}$

$$= \frac{2}{L} \cdot V_0 \int_0^{\pi/2} \sin^2(u) \cdot \frac{L}{\pi}\, du$$

$$= \frac{2V_0}{\pi} \int_0^{\pi/2} \sin^2(u)\, du = \frac{2V_0}{\pi} \cdot \frac{\pi}{4} = \underline{\underline{\frac{V_0}{2}}}$$

$$\therefore\ E_1 = \frac{\pi^2\hbar^2}{2mL^2} + \frac{V_0}{2} + \mathcal{O}(V_0^2)$$

Now, how about the wave function?

$$\psi_1^1(x) = \sum_{m\neq 1} \frac{\langle \psi_m^0 | \hat{H}' | \psi_1^0 \rangle}{E_1 - E_m} \cdot \psi_m^0(x)$$

Calculate $\langle \psi_m^0 | \hat{H}' | \psi_1^0 \rangle = \int_0^{L/2} \psi_m^0(x)^* V_0 \psi_1^0(x)\,dx$

$$= V_0 \cdot \frac{2}{L} \int_0^{L/2} \sin\left(\frac{m\pi x}{L}\right) \sin\left(\frac{\pi x}{L}\right) dx$$

Let $u = \frac{\pi x}{L}$ $du = \frac{\pi dx}{L}$ $\Rightarrow$ $\frac{2V_0}{L} \cdot \frac{L}{\pi} \underbrace{\int_0^{\pi/2} \sin(mu)\sin(u)\,du}_{\frac{m}{1-m^2}\cos\left(\frac{m\pi}{2}\right)}$

$$\langle \psi_m^0 | \hat{H}' | \psi_1^0 \rangle = \frac{2V_0}{\pi} \cdot \frac{m}{1-m^2} \cos\left(\frac{m\pi}{2}\right).$$

Note $\cos\left(\frac{m\pi}{2}\right) = \begin{cases} 0 & \text{if } m \text{ is odd} \\ (-1)^{m/2} & \text{if } m \text{ is even.} \end{cases}$

$$\therefore \psi_1^1(x) = \sum_{m=2,4,6}^{\infty} \cdot \frac{\frac{2V_0}{\pi}\left(\frac{m}{1-m^2}\right)(-1)^{m/2}}{\frac{\pi^2\hbar^2}{2mL^2} - \frac{m^2\pi^2\hbar^2}{2mL^2}} \cdot \sqrt{\frac{2}{L}} \cdot \sin\left(\frac{m\pi x}{L}\right)$$

$$= \frac{4mL^2 V_0}{\pi^3\hbar^2} \sqrt{\frac{2}{L}} \sum_{m=2,4,6\ldots} (-1)^{m/2} \frac{m}{(m^2-1)^2} \sin\left(\frac{m\pi x}{L}\right)$$

In dimensionless units, $z_0 \equiv \frac{V_0}{\pi^2\hbar^2/2mL^2}$ $u = \frac{x}{L}$

$$\psi_1^1(u) = \frac{2z_0}{\pi} \sqrt{\frac{2}{L}} \sum_{m=2,4,6,\ldots} (-1)^{\frac{m}{2}} \frac{m}{(m^2-1)^2} \sin(m\pi u)$$

In all, our approximate wave function and energy is:

$$\psi_1(u) = \sqrt{\frac{2}{L}} \cdot \left[\sin(\pi u) + \frac{2 z_0}{\pi} \cdot \sum_{n=2,4,6\ldots} \frac{(-1)^{n/2}\, n}{(n^2-1)^2} \cdot \sin(n\pi u) \right]$$

where $u = x/L$ and $z_0 = \dfrac{V_0}{\pi^2\hbar^2/2mL^2}$

$$E_1 = \frac{\pi^2\hbar^2}{2mL^2} + \frac{V_0}{2} = \frac{\pi^2\hbar^2}{2mL^2}\left[1 + \frac{z_0}{2} \right]$$

It is actually possible to study this system exactly (see Appendix for details). I chose $z_0 = 1.5$, so $V_0 = 3\pi^2\hbar^2/2mL^2$. The "exact" ground state energy is

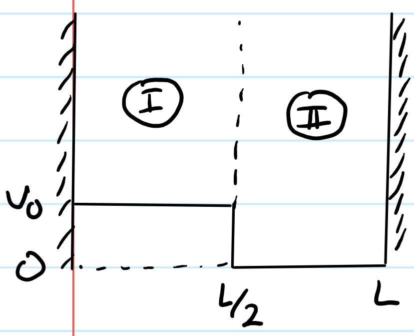
$$E_1^{exact} = \frac{\pi^2\hbar^2}{2mL^2}(1.615)$$

$$E_1^{approx} = E_1^0 + E_1^1 = \frac{\pi^2\hbar^2}{2mL^2} \cdot (1.75)$$ about 8% error.

The wave function is very accurate!

Appendix - "Exact" solution

For comparison, the infinite square well with uneven bottom can be solved "exactly" using techniques learned earlier:



The Schrödinger equation in the two regions are

$$-\frac{\hbar^2}{2m}\psi_I''(x) + V_0\,\psi_I(x) = E\,\psi_I(x)$$

$$-\frac{\hbar^2}{2m}\psi_{II}''(x) = E\,\psi_{II}(x)$$

$$k \equiv \sqrt{\frac{2mE}{\hbar^2}} \qquad q \equiv \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$$

$$\psi_I(x) = A\cos(qx) + B\sin(qx)$$

$$\psi_{II}(x) = C\cos(kx) + D\sin(kx)$$

Boundary conditions: $\psi_I(0) = 0$, $\psi_{II}(L) = 0$

$\Rightarrow A = 0$ and $C\cdot\cos(kL) + D\sin(kL) = 0$

$$C = -D\tan(kL)$$

$$\psi_I(x) = B\sin(qx)$$

$$\psi_{II}(x) = D\sin(kx) - \tan(kL)\cos(kx)$$

$$= \frac{D}{\cos(kL)}\left[\sin(kx)\cos(kL) - \sin(kL)\cos(kx)\right] = F\sin(k(x-L))$$

$\frac{D}{\cos(kL)}$ ← call this F

Wave function & derivative must be continuous at $x = \frac{L}{2}$

① $\psi_I(\frac{L}{2}) = \psi_{II}(\frac{L}{2}) \Rightarrow B\sin(\frac{qL}{2}) = F\sin(-\frac{kL}{2}) = -F\sin(\frac{kL}{2})$

② $\psi_I'(\frac{L}{2}) = \psi_{II}'(\frac{L}{2}) \Rightarrow Bq\cos(\frac{qL}{2}) = Fk\cos(-\frac{kL}{2}) = Fk\cos(\frac{kL}{2})$

Dividing these two gives
$$\frac{\tan(\frac{qL}{2})}{q} = -\frac{\tan(\frac{kL}{2})}{k}$$

this equation determines the energy, E, assuming V_0, m, L are given.

Appendix - "Exact" solution

$$\frac{\tan\left(\frac{qL}{2}\right)}{q} = -\frac{\tan\left(\frac{kL}{2}\right)}{k}$$ ← Determines E, k, q

and

$$\psi(x) = \begin{cases} B\cdot\sin(qx) & 0<x<L/2 \\ B\dfrac{\sin(qL/2)}{\sin(kL/2)}\sin(k(L-x)) & L/2<x<L \end{cases}$$

Define $A \equiv \dfrac{B}{\sin(kL/2)}$ to get

$$\psi(x) = \begin{cases} A\cdot\sin(kL/2)\sin(qx) & 0<x<L/2 \\ A\sin(qL/2)\sin(k(L-x)) & L/2<x<L \end{cases}$$

A must be determined by normalization.

Now, determine ground state energy: $\tan\left(\frac{kL}{2}\right) = -\frac{k}{q}\tan\left(\frac{qL}{2}\right)$

$$\tan\left(\frac{L}{2}\sqrt{\frac{2mE}{\hbar^2}}\right) = -\sqrt{\frac{E}{E-V_0}}\tan\left(\frac{L}{2}\sqrt{\frac{2m(E-V_0)}{\hbar^2}}\right)$$

Let's measure E in units of $\frac{\pi^2\hbar^2}{2mL^2}$ $\quad E = z\left(\frac{\pi^2\hbar^2}{2mL^2}\right)$ $\quad V_0 = z_0\left(\frac{\pi^2\hbar^2}{2mL^2}\right)$

$$\therefore \frac{2mE}{\hbar^2} = \frac{\pi^2 z}{L^2}$$

$$k = \sqrt{\frac{2mE}{\hbar^2}} = \frac{\pi}{L}\cdot\sqrt{z} \qquad q = \frac{\pi}{L}\sqrt{z-z_0}$$

$\therefore$

$$\tan\left(\frac{\pi}{2}\sqrt{z}\right) = -\sqrt{\frac{z}{z-z_0}}\tan\left(\frac{\pi}{2}\sqrt{z-z_0}\right)$$

$$\psi(u) = \begin{cases} A\cdot\sin\left(\frac{\pi}{2}\sqrt{z}\right)\sin\left(\pi\sqrt{z-z_0}\cdot u\right) & 0\le u\le\frac{1}{2} \\ A\sin\left(\frac{\pi}{2}\sqrt{z-z_0}\right)\sin\left(\pi\sqrt{z}(1-u)\right) & \frac{1}{2}\le u\le 1 \end{cases}$$

$$u \equiv x/L$$

Appendix - Mathematica Output

Here we investigate the infinite square well which has an uneven bottom. V (x) = V0 for 0 < x < L/2, and V (x) = 0 for L/2 < x < L.

```
z0 := 1.5 (*Height of V0 in units of π²h²/2 m L²*)

(*z = E in units of π²h²/2 m L².  If z0 = 0, then z = 1*)
(*The transcendental equation which determines z is*)
zsoln =
```

$$\text{FindRoot}\left[\text{Sin}\left[\frac{\pi}{2}\sqrt{z}\right]\text{Cos}\left[\frac{\pi}{2}\sqrt{z-z0}\right]+\sqrt{\frac{z}{z-z0}}\,\text{Sin}\left[\frac{\pi}{2}\sqrt{z-z0}\right]\text{Cos}\left[\frac{\pi}{2}\sqrt{z}\right],\{z,1.6\}\right]$$

```
zz = z /. zsoln;
{z → 1.61467}

(*The unnormalized wave function in dimensionless form is: *)
(*Here u = x/L*)
```

$$\psi\text{exact}[u\_] := \text{Piecewise}\left[\left\{\left\{A*\text{Sin}\left[\frac{\pi}{2}\sqrt{zz}\right]\text{Sin}\left[\pi\sqrt{zz-z0}\,u\right],0<u<1/2\right\},\left\{A*\text{Sin}\left[\frac{\pi}{2}\sqrt{zz-z0}\right]\text{Sin}\left[\pi\sqrt{zz}\,(1-u)\right],1/2<u<1\right\}\right\}\right]$$

```
(*Normalize*)
Asoln = Solve[1 == Integrate[ψexact[u]^2, {u, 0, 1}], A]
{{A → -2.96967}, {A → 2.96967}}

(*Perturbation Theory Result*)
```

$$\psi\text{Approx}[u\_] = \sqrt{2}\left(\text{Sin}[\pi u]+\frac{2\,z0}{\pi}\text{Sum}\left[\frac{n*(-1)^{n/2}}{(1-n^2)^2}\text{Sin}[n\pi u],\{n,2,10,2\}\right]\right);$$

```
Plot[{(ψexact[u] /. Asoln[[2]]), √2 Sin[π u], ψApprox[u]},
 {u, 0, 1}, Frame → True, LabelStyle → {16, Bold},
 FrameLabel → {"x/L", "ψ(x) * √L", "Ground State in an Uneven Infinite Square Well"},
 PlotLegends → {"Exact", "ψ⁰", "ψ⁰+ψ¹"}]
```