

8.3 Perturbation theory

Slides: Video 8.3.4 Applying
perturbation theory

Text reference: Quantum Mechanics
for Scientists and Engineers

Section 6.3 (starting at “Example
of well with field”)





Perturbation theory



Applying perturbation theory

Quantum mechanics for scientists and engineers

David Miller

Example of a well with field

We write the Hamiltonian as the sum of

the unperturbed Hamiltonian

which is, in the well, in our dimensionless units

$$\hat{H}_o = -\frac{1}{\pi^2} \frac{d^2}{d\xi^2}$$

and the perturbing Hamiltonian

$$\hat{H}_p = f(\xi - 1/2)$$

where again we take $f = 3$ for an explicit calculation

First order energy correction

In first order, the energy shift with applied field is

$$\begin{aligned} E^{(1)} &= \langle \psi_m | \hat{H}_p | \psi_m \rangle = \int_0^1 \sqrt{2} \sin(m\pi\xi) (\xi - 1/2) \sqrt{2} \sin(m\pi\xi) d\xi \\ &= 2 \int_0^1 (\xi - 1/2) \sin^2(m\pi\xi) d\xi = 0 \end{aligned}$$

The integrals here are zero for all m

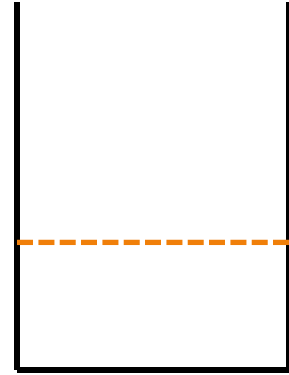
because the sine squared function is even with respect to the center of the well

whereas $(\xi - 1/2)$ is odd

Hence, for this particular problem there is no first order energy correction

First order energy correction

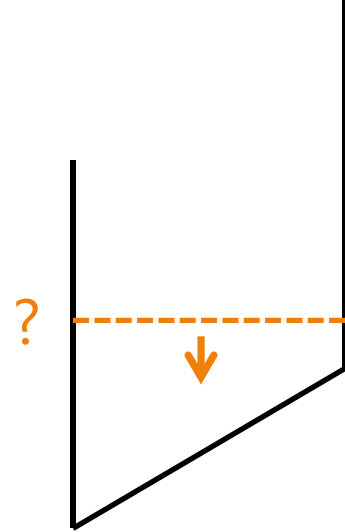
There no first order energy correction
because of symmetry



First order energy correction

There no first order energy correction
because of symmetry

If the energy changed
proportionately with applied field

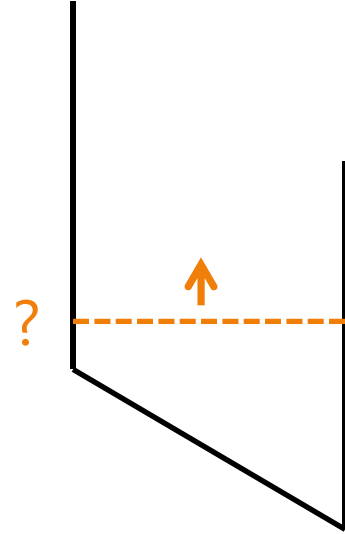


First order energy correction

There no first order energy correction
because of symmetry

If the energy changed
proportionately with applied field
changing field direction (or sign)
would change the energy
correction sign

But, by symmetry here
the energy change cannot depend
field direction



Matrix elements for perturbation calculations

The general matrix elements that we will need for further perturbation calculations are

$$H_{puv} = \langle \psi_u | \hat{H}_p | \psi_v \rangle = \int_0^1 \sqrt{2} \sin(u\pi\xi) (\xi - 1/2) \sqrt{2} \sin(v\pi\xi) d\xi$$

In general we need u and v to have opposite parity

i.e., if one is odd, the other must be even

for these matrix elements to be non-zero

since otherwise

the overall integrand is odd about $\xi = 1/2$

First order correction to the wavefunction

We calculate the first order wavefunction correction
for the first state, i.e., for $m = 1$

$$\left| \phi^{(1)} \right\rangle = \sum_{n=2}^q a_n^{(1)} \left| \psi_n \right\rangle \quad a_i^{(1)} = \frac{\langle \psi_i | \hat{H}_p | \psi_1 \rangle}{\varepsilon_{o1} - \varepsilon_{oi}}$$

where $\varepsilon_{on} = n^2$ are the energies of the unperturbed states, and

q is a finite number we must choose in practice

Here, we chose $q = 6$

though a smaller number would likely be quite accurate

First order correction to the wavefunction

Explicitly, for the expansion coefficients

$$a_i^{(1)} = \langle \psi_i | \hat{H}_p | \psi_1 \rangle / (\varepsilon_{o1} - \varepsilon_{oi})$$

for 3 units of field

we have numerically

$$a_2^{(1)} \simeq 0.180 \quad a_3^{(1)} = 0 \quad a_4^{(1)} \simeq 0.003$$

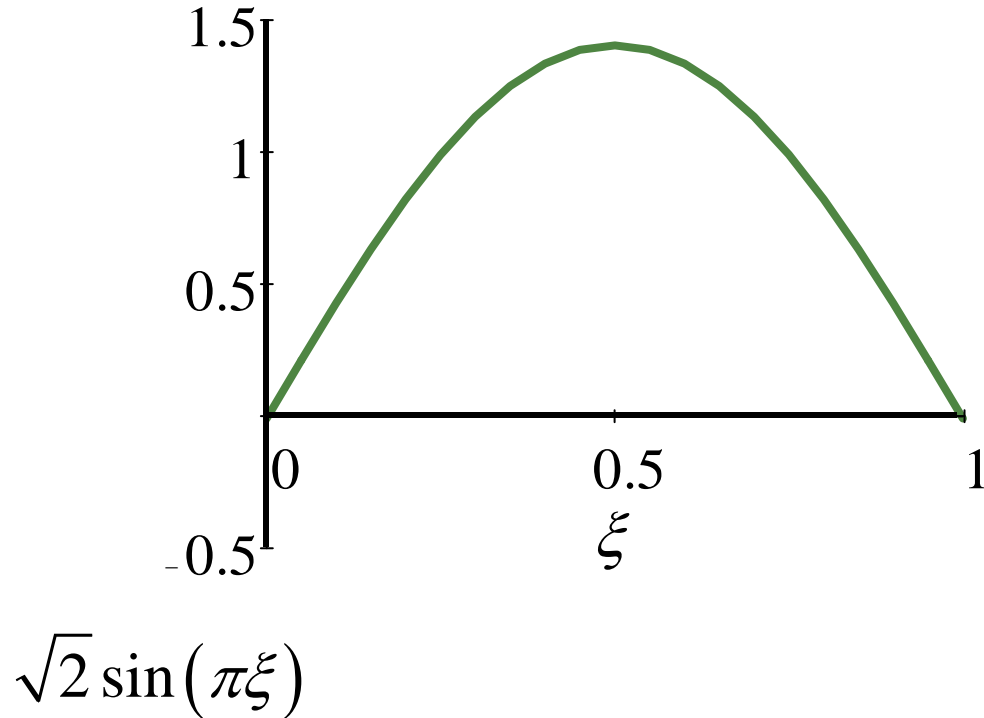
Here

the value of 0.180 for $a_2^{(1)}$

compares closely with the value of 0.174 obtained
above in the finite basis subset method

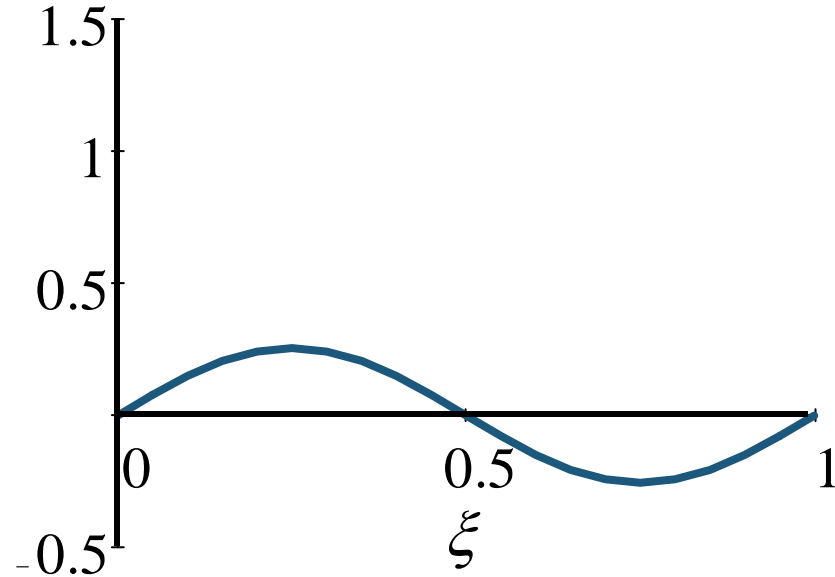
First order correction to the wavefunction

We sum the zero-order (unperturbed) wavefunction



First order correction to the wavefunction

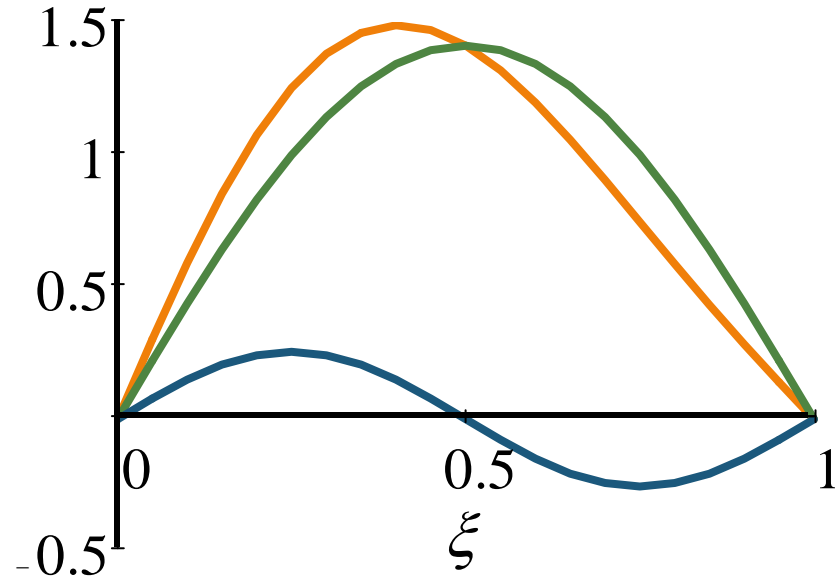
and the first order correction part from the second basis function



$$0.180\sqrt{2} \sin(2\pi\xi)$$

First order correction to the wavefunction

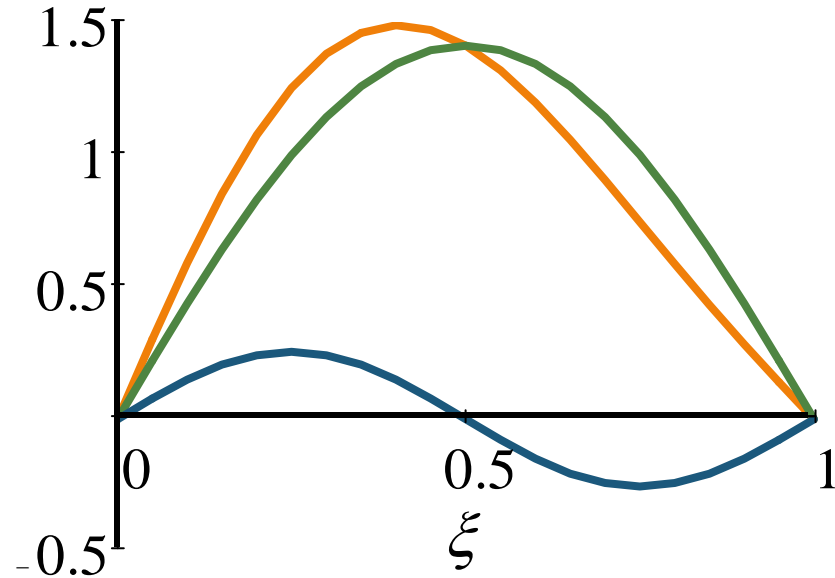
To get our approximate wavefunction solution



$$\psi(\xi) \simeq \sqrt{2} \sin(\pi\xi) + 0.180\sqrt{2} \sin(2\pi\xi)$$

First order correction to the wavefunction

Adding the next correction makes negligible difference



$$\psi(\xi) \simeq \sqrt{2} \sin(\pi\xi) + 0.180\sqrt{2} \sin(2\pi\xi) + 0.003\sqrt{2} \sin(4\pi\xi)$$

Second order energy correction

Since the first order correction to the energy was zero
to get a perturbation correction to the energy
we go to second order

Explicitly, we have
$$E^{(2)} = \langle \psi_1 | \hat{H}_p | \phi^{(1)} \rangle = \sum_{n=2}^q \frac{|\langle \psi_n | \hat{H}_p | \psi_1 \rangle|^2}{E_1 - E_n}$$

which numerically here gives $E^{(2)} = -0.0975$

or a total energy of $\eta_1 \simeq \varepsilon_1 + E^{(1)} + E^{(2)} = 0.9025$

which compares with the result of

$\eta_1 = 0.904$ from the finite basis subset method

Approximate analytic formulas

Note that $E^{(2)}$

is analytically proportional to the square of the field f^2

$$\begin{aligned} E^{(2)} &= \sum_{n=2}^q \frac{|\langle \psi_n | \hat{H}_p | \psi_1 \rangle|^2}{E_1 - E_n} = \sum_{n=2}^q \frac{|\langle \psi_n | f(\xi - 1/2) | \psi_1 \rangle|^2}{E_1 - E_n} \\ &= f^2 \sum_{n=2}^q \frac{|\langle \psi_n | (\xi - 1/2) | \psi_1 \rangle|^2}{E_1 - E_n} \end{aligned}$$

Approximate analytic formulas

Hence perturbation theory

gives an approximate analytic result for the energy
which we can now use for any field

Explicitly, we can write for the energy of the first state
in dimensionless units

$$\eta_1 \cong \varepsilon_1 - 0.0108f^2$$

This typical kind of result from perturbation theory
gives us an approximate analytic formula
valid for small perturbations

Approximate analytic formulas

Similarly, for the wavefunction

the correction is approximately proportional to field
for example with expansion coefficient

$$a_i^{(1)} = \frac{\langle \psi_i | \hat{H}_p | \psi_m \rangle}{E_m - E_i} = f \frac{\langle \psi_i | (\xi - 1/2) | \psi_m \rangle}{E_m - E_i}$$

So, keeping only the dominant contribution from the second-state wavefunction in our example

we would have the approximate formula for small f

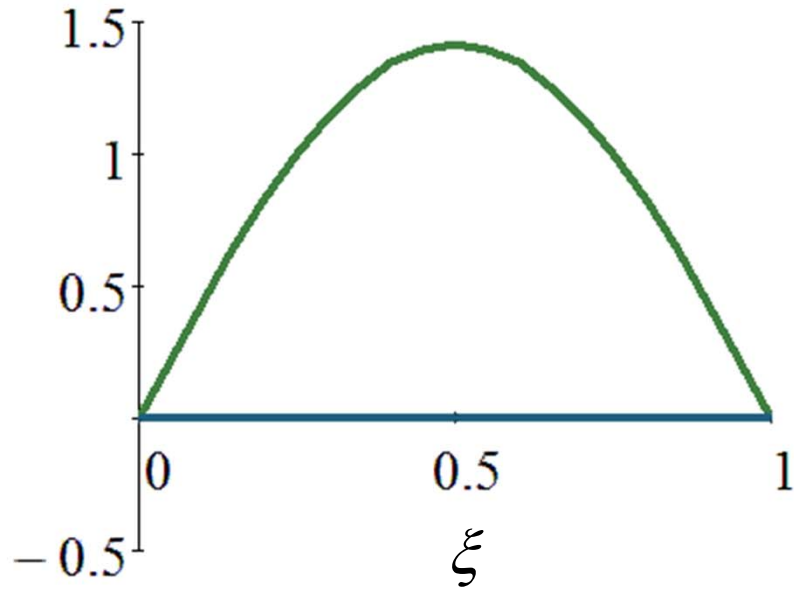
$$\phi(\xi) \cong \sqrt{2} \sin(\pi\xi) + 0.06f\sqrt{2} \sin(2\pi\xi)$$

(This is not quite normalized, though that could be done)

Approximate analytic results

Wavefunction

Field = 0



Energy

