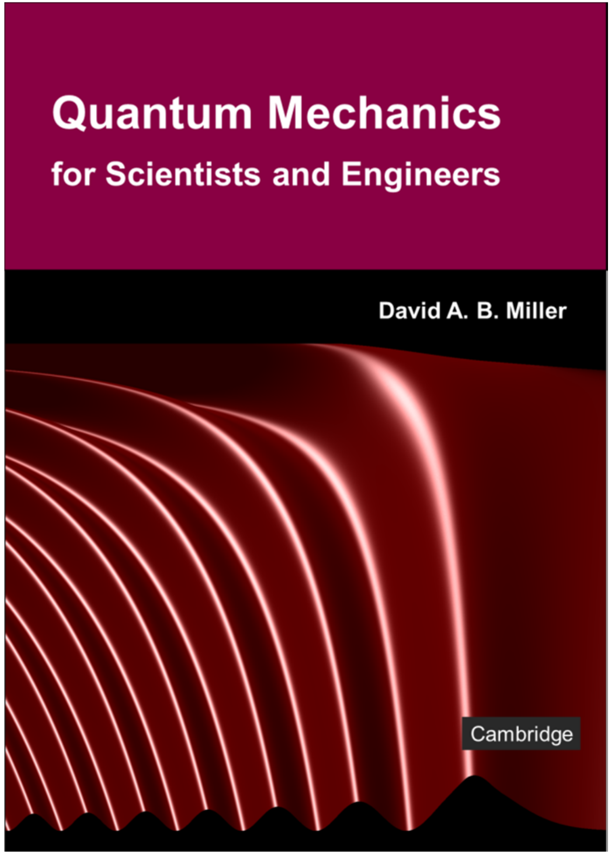
8.3 Perturbation theory

Slides: Video 8.3.1 Constructing perturbation theory

Text reference: Quantum Mechanics for Scientists and Engineers

Section 6.3 (up to "First order perturbation theory")



Perturbation theory

Constructing perturbation theory

Quantum mechanics for scientists and engineers

David Miller

Time-independent perturbation theory

Presume some unperturbed Hamiltonian $\hat{H}_o$

that has known normalized eigen solutions

i.e., $\hat{H}_0 \left|\psi_n\right\rangle = E_n \left|\psi_n\right\rangle$

We can imagine that our perturbation

could be progressively "turned on"

at least in a mathematical sense

For example

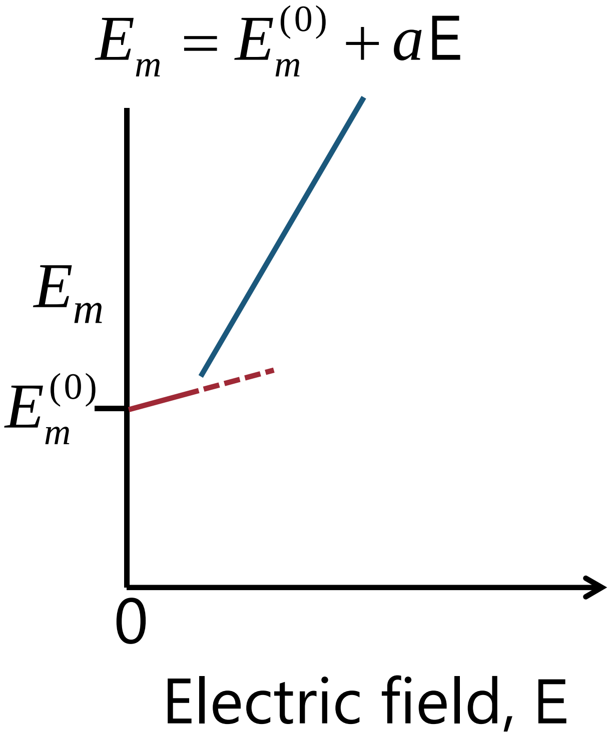
we could be progressively increasing applied field E

from zero to some specific value

Time-independent perturbation theory

We look successively

- for the changes in the solutions
  - for example, for the mth energy eigenvalue E_m
- proportional first to electric field E
  - "first-order corrections"

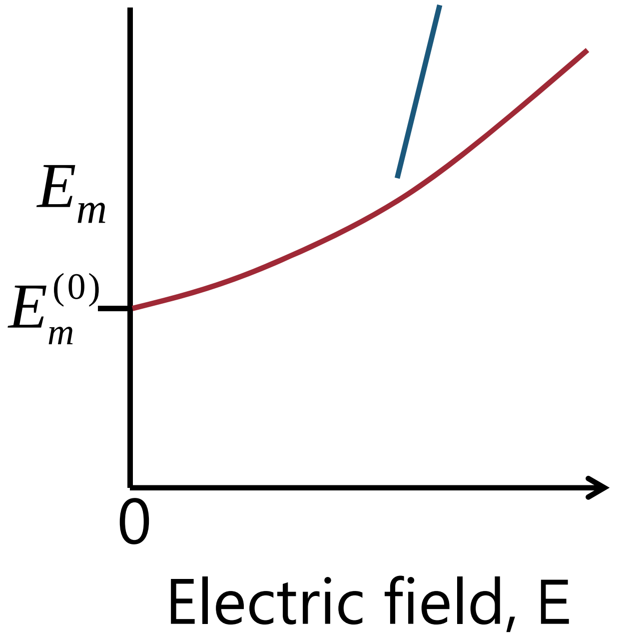


Time-independent perturbation theory

We look successively

- for the changes in the solutions
  - for example, for the mth energy eigenvalue E_m
- proportional first to electric field E
  - "first-order corrections"
- proportional to E^2
  - "second-order corrections"
- and so on

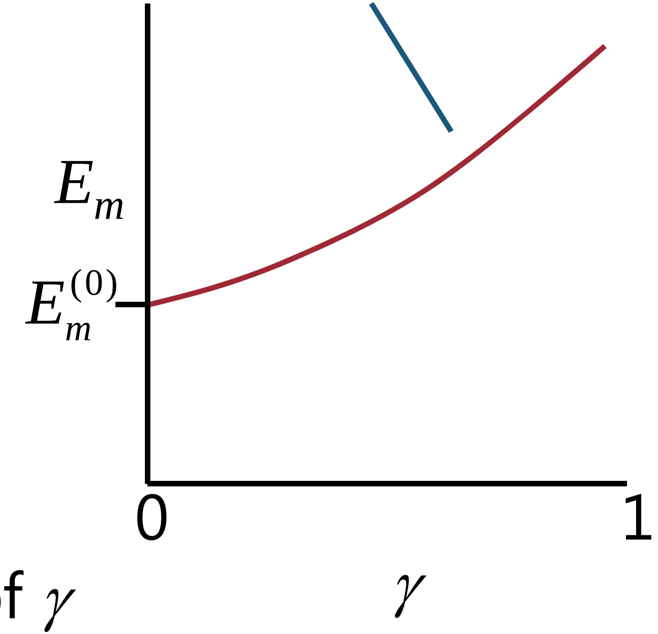
$$E_m = E_m^{(0)} + a\mathsf{E} + b\mathsf{E}^2 + \ldots$$



Time-independent perturbation theory

It is more convenient and general
 if we imagine a specific fixed perturbation (e.g., a field E)
and we mathematically increase a "house-keeping" parameter γ
 from 0 to 1
 so our perturbation is γE
 with E fixed
Now we express changes as orders of γ
 rather than of the field itself

$$E_m = E_m^{(0)} + \gamma E_m^{(1)} + \gamma^2 E_m^{(2)} + \ldots$$



The "house-keeping" parameter γ

So, instead of writing $E_m = E_m^{(0)} + a\mathrm{E} + b\mathrm{E}^2 + \ldots$

we are writing $E_m = E_m^{(0)} + \gamma E_m^{(1)} + \gamma^2 E_m^{(2)} + \ldots$

and instead of working out a and b

we are going to work out parameters

$E_m^{(1)}$ and $E_m^{(2)}$ and so on

These have dimensions of energy

and reflect the "first order" and "second order" corrections to the energy

as a result of the specific perturbation

e.g., a *specific* field E

The "house-keeping" parameter γ

In general, then, we imagine that our perturbed system has some additional term in the Hamiltonian

the "perturbing Hamiltonian" $\hat{H}_p$

In our example case of an infinitely deep potential well

with an applied field

that perturbing Hamiltonian would be $\hat{H}_p = e\text{E}(z - L_z / 2)$

In the theory, we write the perturbing Hamiltonian as $\gamma\hat{H}_p$

using γ to keep track of the order of the corrections

through the powers of γ in the expressions

We can set $\gamma = 1$ at the end if we like

The "house-keeping" parameter γ

So, we could set up the theory using $E_m = E_m^{(0)} + a\mathrm{E} + b\mathrm{E}^2 + \ldots$

in which case we would work out a and b

and some other parameters

But, to make it more general we use

$$E_m = E_m^{(0)} + \gamma E_m^{(1)} + \gamma^2 E_m^{(2)} + \ldots$$

and work out the parameters

$E_m^{(1)}$ and $E_m^{(2)}$ and some other parameters

If this is confusing at first

then just think of γ as the strength of the electric field

in our specific problem

Construction of the orders of perturbation theory

With this way of thinking about the problem mathematically

we can write the perturbed Schrödinger equation as

$$\left(\hat{H}_o + \gamma \hat{H}_p\right)|\phi\rangle = E|\phi\rangle$$

We now presume that we can express

the resulting perturbed eigenfunction and eigenvalue

as power series in this parameter, i.e.,

$$|\phi\rangle = \left|\phi^{(0)}\right\rangle + \gamma\left|\phi^{(1)}\right\rangle + \gamma^2\left|\phi^{(2)}\right\rangle + \gamma^3\left|\phi^{(3)}\right\rangle + \cdots$$

$$E = E^{(0)} + \gamma E^{(1)} + \gamma^2 E^{(2)} + \gamma^3 E^{(3)} + \cdots$$

Construction of the orders of perturbation theory

We now substitute these power series

$$\left|\phi\right\rangle = \left|\phi^{(0)}\right\rangle + \gamma\left|\phi^{(1)}\right\rangle + \gamma^2\left|\phi^{(2)}\right\rangle + \gamma^3\left|\phi^{(3)}\right\rangle + \cdots$$

$$E = E^{(0)} + \gamma E^{(1)} + \gamma^2 E^{(2)} + \gamma^3 E^{(3)} + \cdots$$

into the perturbed Schrödinger equation

$$\left(\hat{H}_o + \gamma\hat{H}_p\right)\left|\phi\right\rangle = E\left|\phi\right\rangle$$

to get

$$\left(\hat{H}_0 + \gamma\hat{H}_p\right)\left(\left|\phi^{(0)}\right\rangle + \gamma\left|\phi^{(1)}\right\rangle + \gamma^2\left|\phi^{(2)}\right\rangle + \cdots\right)$$

$$= \left(E^{(0)} + \gamma E^{(1)} + \gamma^2 E^{(2)} + \cdots\right)\left(\left|\phi^{(0)}\right\rangle + \gamma\left|\phi^{(1)}\right\rangle + \gamma^2\left|\phi^{(2)}\right\rangle + \cdots\right)$$

Construction of the orders of perturbation theory

Now, at any specific point in space, each function $\left|\phi^{(n)}\right\rangle$

and each function $\left(\hat{H}_0 + \gamma \hat{H}_p\right)\left|\phi^{(n)}\right\rangle$

is just some number

So, at any specific point in space, the left hand side of

$$\left(\hat{H}_0 + \gamma \hat{H}_p\right)\left(\left|\phi^{(0)}\right\rangle + \gamma\left|\phi^{(1)}\right\rangle + \gamma^2\left|\phi^{(2)}\right\rangle + \cdots\right)$$

$$= \left(E^{(0)} + \gamma E^{(1)} + \gamma^2 E^{(2)} + \cdots\right)\left(\left|\phi^{(0)}\right\rangle + \gamma\left|\phi^{(1)}\right\rangle + \gamma^2\left|\phi^{(2)}\right\rangle + \cdots\right)$$

is just a power series in γ, e.g., $a_0 + a_1\gamma + a_2\gamma^2 + a_3\gamma^3 + \cdots$

and so is the right hand side, e.g., $b_0 + b_1\gamma + b_2\gamma^2 + b_3\gamma^3 + \cdots$

Construction of the orders of perturbation theory

Because a power series expansion is unique

the only way the equality of two power series can work

$$a_0 + a_1\gamma + a_2\gamma^2 + a_3\gamma^3 + \cdots = b_0 + b_1\gamma + b_2\gamma^2 + b_3\gamma^3 + \cdots$$

for every value of γ within some convergence range

e.g., 0 to 1

is if the terms are equal, one by one, i.e.,

$$a_0 = b_0 \quad a_1 = b_1 \quad a_2 = b_2 \quad a_3 = b_3$$

and so on

Construction of the orders of perturbation theory

Hence, in

$$\left(\hat{H}_0 + \gamma \hat{H}_p\right)\left(\left|\phi^{(0)}\right\rangle + \gamma\left|\phi^{(1)}\right\rangle + \gamma^2\left|\phi^{(2)}\right\rangle + \cdots\right)$$

$$= \left(E^{(0)} + \gamma E^{(1)} + \gamma^2 E^{(2)} + \cdots\right)\left(\left|\phi^{(0)}\right\rangle + \gamma\left|\phi^{(1)}\right\rangle + \gamma^2\left|\phi^{(2)}\right\rangle + \cdots\right)$$

we can equate each term with a specific power of γ

and hence obtain

a progressive set of equations

which we can solve to evaluate corrections

to whatever order we wish

Progressive set of perturbation theory equations

In $\left(\hat{H}_0 + \gamma\hat{H}_p\right)\left(\left|\phi^{(0)}\right\rangle + \gamma\left|\phi^{(1)}\right\rangle + \gamma^2\left|\phi^{(2)}\right\rangle + \cdots\right)$

$$= \left(E^{(0)} + \gamma E^{(1)} + \gamma^2 E^{(2)} + \cdots\right)\left(\left|\phi^{(0)}\right\rangle + \gamma\left|\phi^{(1)}\right\rangle + \gamma^2\left|\phi^{(2)}\right\rangle + \cdots\right)$$

equating terms in γ^0, i.e., terms without γ

gives the "zeroth" order equation $\hat{H}_o\left|\phi^{(0)}\right\rangle = E^{(0)}\left|\phi^{(0)}\right\rangle$

i.e., the unperturbed Hamiltonian equation

with eigenfunctions $\left|\psi_n\right\rangle$ and eigenvalues E_n

So if we now presume we start in a specific eigenstate $\left|\psi_m\right\rangle$

we write $\left|\psi_m\right\rangle$ and E_m

instead of $\left|\phi^{(0)}\right\rangle$ and $E^{(0)}$

Progressive set of perturbation theory equations

So, with $\left(\hat{H}_0 + \gamma \hat{H}_p\right)\left(|\psi_m\rangle + \gamma\left|\phi^{(1)}\right\rangle + \gamma^2\left|\phi^{(2)}\right\rangle + \cdots\right)$

$$= \left(E_m + \gamma E^{(1)} + \gamma^2 E^{(2)} + \cdots\right)\left(|\psi_m\rangle + \gamma\left|\phi^{(1)}\right\rangle + \gamma^2\left|\phi^{(2)}\right\rangle + \cdots\right)$$

we get a progressive set of equations

each equating a different power of γ

$$\hat{H}_o|\psi_m\rangle = E_m|\psi_m\rangle$$

$$\hat{H}_o\left|\phi^{(1)}\right\rangle + \hat{H}_p|\psi_m\rangle = E_m\left|\phi^{(1)}\right\rangle + E^{(1)}|\psi_m\rangle$$

$$\hat{H}_o\left|\phi^{(2)}\right\rangle + \hat{H}_p\left|\phi^{(1)}\right\rangle = E_m\left|\phi^{(2)}\right\rangle + E^{(1)}\left|\phi^{(1)}\right\rangle + E^{(2)}|\psi_m\rangle$$

and so on

Progressive set of perturbation theory equations

We can rewrite these equations as

$$\hat{H}_o\left|\psi_m\right\rangle = E_m\left|\psi_m\right\rangle \quad \rightarrow \quad \boxed{\left(\hat{H}_o - E_m\right)\left|\psi_m\right\rangle = 0}$$

$$\hat{H}_o\left|\phi^{(1)}\right\rangle + \hat{H}_p\left|\psi_m\right\rangle = E_m\left|\phi^{(1)}\right\rangle + E^{(1)}\left|\psi_m\right\rangle$$

$$\rightarrow \quad \boxed{\left(\hat{H}_o - E_m\right)\left|\phi^{(1)}\right\rangle = \left(E^{(1)} - \hat{H}_p\right)\left|\psi_m\right\rangle}$$

$$\hat{H}_o\left|\phi^{(2)}\right\rangle + \hat{H}_p\left|\phi^{(1)}\right\rangle = E_m\left|\phi^{(2)}\right\rangle + E^{(1)}\left|\phi^{(1)}\right\rangle + E^{(2)}\left|\psi_m\right\rangle$$

$$\rightarrow \quad \boxed{\left(\hat{H}_o - E_m\right)\left|\phi^{(2)}\right\rangle = \left(E^{(1)} - \hat{H}_p\right)\left|\phi^{(1)}\right\rangle + E^{(2)}\left|\psi_m\right\rangle}$$

and so on