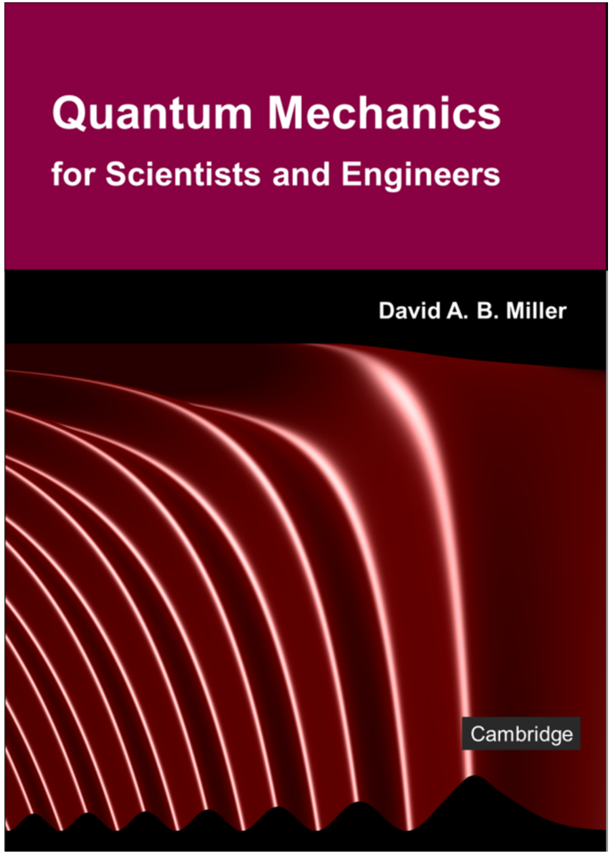
9.2 Time-dependent perturbation theory

Slides: Video 9.2.1 Time-dependent perturbation basics

Text reference: Quantum Mechanics for Scientists and Engineers

Section 7.1



Time-dependent perturbation theory

Time-dependent perturbation basics

Quantum mechanics for scientists and engineers

David Miller

Time-dependent perturbation theory

For time-dependent problems

consider some time-dependent perturbation $\hat{H}_p(t)$

to an unperturbed Hamiltonian $\hat{H}_o$

that is itself not dependent on time

The total Hamiltonian is then

$$\hat{H} = \hat{H}_o + \hat{H}_p(t)$$

To deal with such a situation

we use the time-dependent Schrödinger equation

$$i\hbar \frac{\partial}{\partial t}|\Psi\rangle = \hat{H}|\Psi\rangle$$

where now the ket $|\Psi\rangle$ is generally time-varying

Time-dependent perturbation theory

With $|\psi_n\rangle$ and E_n as the energy eigenfunctions and eigenvalues of the time-independent equation

$$\hat{H}_o|\psi_n\rangle = E_n|\psi_n\rangle$$

we expand the solution

of the time-dependent Schrödinger equation as

$$|\Psi\rangle = \sum_n a_n(t)\exp(-iE_n t/\hbar)|\psi_n\rangle$$

Note we included the time-dependent factor $\exp(-iE_n t/\hbar)$

explicitly in the expansion

leaving the time dependence of $a_n(t)$

to deal only with the additional changes

Time-dependent perturbation theory

Now we substitute $\left|\Psi\right\rangle = \sum_n a_n(t)\exp(-iE_n t/\hbar)\left|\psi_n\right\rangle$

into the Schrödinger equation $i\hbar\frac{\partial}{\partial t}\left|\Psi\right\rangle = \hat{H}\left|\Psi\right\rangle$ gives

$$\sum_n \left(i\hbar\dot{a}_n + a_n E_n\right)\exp(-iE_n t/\hbar)\left|\psi_n\right\rangle$$

$$= \sum_n a_n\left(\hat{H}_o + \hat{H}_p(t)\right)\exp(-iE_n t/\hbar)\left|\psi_n\right\rangle$$ where $\dot{a}_n \equiv \frac{\partial a_n}{\partial t}$

Replacing $\hat{H}_o\left|\psi_n\right\rangle$ with $E_n\left|\psi_n\right\rangle$ and cancelling gives

$$\sum_n i\hbar\dot{a}_n \exp(-iE_n t/\hbar)\left|\psi_n\right\rangle = \sum_n a_n\hat{H}_p(t)\exp(-iE_n t/\hbar)\left|\psi_n\right\rangle$$

Time-dependent perturbation theory

Now premultiplying

$$\sum_n i\hbar \dot{a}_n \exp\left(-iE_n t/\hbar\right)\left|\psi_n\right\rangle = \sum_n a_n \hat{H}_p(t)\exp\left(-iE_n t/\hbar\right)\left|\psi_n\right\rangle$$

by $\left\langle\psi_q\right|$ on both sides leads to

$$i\hbar \dot{a}_q(t)\exp\left(-iE_q t/\hbar\right) = \sum_n a_n(t)\exp\left(-iE_n t/\hbar\right)\left\langle\psi_q\right|\hat{H}_p(t)\left|\psi_n\right\rangle$$

We have made no approximations so far

This is merely a restatement of Schrödinger's time-dependent equation

$$i\hbar\frac{\partial}{\partial t}\left|\Psi\right\rangle = \hat{H}\left|\Psi\right\rangle$$

Time-dependent perturbation theory

Now we consider a perturbation series

We introduce the expansion parameter γ as before

now writing our perturbation as $\gamma \hat{H}_p$

As before, we can set this to 1 at the end

We now express the expansion coefficients a_n as a power series

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

and we substitute this expansion into

$$i\hbar \dot{a}_q(t)\exp(-iE_q t/\hbar) = \sum_n a_n(t)\exp(-iE_n t/\hbar)\langle \psi_q | \gamma \hat{H}_p(t) | \psi_n \rangle$$

where we now have $\gamma \hat{H}_p$ instead of just $\hat{H}_p$

Time-dependent perturbation theory

In
$$i\hbar\dot{a}_q(t)\exp\left(-iE_q t/\hbar\right)=\sum_n a_n(t)\exp\left(-iE_n t/\hbar\right)\left\langle\psi_q\left|\gamma\hat{H}_p(t)\right|\psi_n\right\rangle$$

equating powers of γ on both sides

first we obtain the zero order term

$$\dot{a}_q^{(0)}(t)=0$$

The zero order solution simply corresponds to the unperturbed solution

and hence there is no change in the expansion coefficients in time to zero order

Time-dependent perturbation theory

With $a_n = a_n^{(0)} + \gamma a_n^{(1)} + \gamma^2 a_n^{(2)} + \cdots$ and

$$i\hbar \dot{a}_q(t)\exp\left(-iE_q t/\hbar\right) = \sum_n a_n(t)\exp\left(-iE_n t/\hbar\right)\left\langle \psi_q \middle| \gamma \hat{H}_p(t) \middle| \psi_n \right\rangle$$

for the first order term we have

$$\dot{a}_q^{(1)}(t) = \frac{1}{i\hbar}\sum_n a_n^{(0)} \exp\left(i\omega_{qn} t\right)\left\langle \psi_q \middle| \hat{H}_p(t) \middle| \psi_n \right\rangle$$

where we have introduced the notation

$$\omega_{qn} = \left(E_q - E_n\right)/\hbar$$

Time-dependent perturbation theory

Note here in $\dot{a}_q^{(1)}(t) = \frac{1}{i\hbar}\sum_n a_n^{(0)} \exp(i\omega_{qn}t)\langle\psi_q|\hat{H}_p(t)|\psi_n\rangle$

we already know tha the $a_n^{(0)}$ are all constants

They give the "starting" state of the system at $t = 0$

We note now that, if we know

the starting state, the perturbing potential and

the unperturbed eigenvalues and eigenfunctions

we can integrate to obtain

the first order, time-dependent correction, $a_q^{(1)}(t)$

to the expansion coefficients

Time-dependent perturbation theory

After integrating $\dot{a}_q^{(1)}(t) = \frac{1}{i\hbar}\sum_n a_n^{(0)} \exp(i\omega_{qn}t)\langle\psi_q|\hat{H}_p(t)|\psi_n\rangle$

we know the new approximate expansion coefficients

$$a_q \simeq a_q^{(0)} + a_q^{(1)}(t)$$

so we know the new wavefunction

and can calculate the behavior of the system

from this new wavefunction

Time-dependent perturbation theory

We can proceed to higher order in this time-dependent perturbation theory

Equating powers of progressively higher order gives

$$\dot{a}_q^{(p+1)}(t) = \frac{1}{i\hbar}\sum_n a_n^{(p)} \exp(i\omega_{qn}t)\langle\psi_q|\hat{H}_p(t)|\psi_n\rangle$$

We see that this perturbation theory is also a method of successive approximations

just like the time-independent perturbation theory

We calculate each higher order correction

from the preceding correction