Lecture 18

Time-dependent perturbation theory
So far, we have focused on quantum mechanics of systems described by Hamiltonians that are *time-independent*.

In such cases, time dependence of wavefunction developed through time-evolution operator, $\hat{U} = e^{-i\hat{H}t/\hbar}$, i.e. for $\hat{H}|n\rangle = E_n|n\rangle$,

$$|\psi(t)\rangle = e^{-i\hat{H}t/\hbar} |\psi(0)\rangle = \sum_n e^{-iE_nt/\hbar} c_n(0)|n\rangle$$

Although suitable for closed quantum systems, formalism fails to describe interaction with an external environment, e.g. EM field.

In such cases, more convenient to describe “induced” interactions of small isolated system, $\hat{H}_0$, through time-dependent interaction $V(t)$.

In this lecture, we will develop a formalism to treat such time-dependent perturbations.
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In this lecture, we will develop a formalism to treat such time-dependent perturbations.
Time-dependent perturbation theory: outline

- Time-dependent potentials: general formalism
- Time-dependent perturbation theory
- “Sudden” perturbation
- Harmonic perturbations: Fermi’s Golden Rule
Consider Hamiltonian \( \hat{H}(t) = \hat{H}_0 + V(t) \), where all time dependence enters through the potential \( V(t) \).

So far, we have focused on Schrödinger representation, where dynamics specified by time-dependent wavefunction,

\[
i\hbar \partial_t |\psi(t)\rangle_S = \hat{H} |\psi(t)\rangle_S
\]

However, to develop time-dependent perturbation theory for \( \hat{H}(t) = \hat{H}_0 + V(t) \), it is convenient to turn to a new representation known as the Interaction representation:

\[
|\psi(t)\rangle_I = e^{i\hat{H}_0 t/\hbar} |\psi(t)\rangle_S,
|\psi(0)\rangle_I = |\psi(0)\rangle_S
\]
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$$|\psi(t)\rangle_I = e^{i\hat{H}_0 t/\hbar} |\psi(t)\rangle_S, \quad |\psi(0)\rangle_I = |\psi(0)\rangle_S$$
In the interaction representation, wavefunction obeys the following equation of motion:

\[
\begin{align*}
  i\hbar \partial_t |\psi(t)\rangle_I &= e^{i\hat{H}_0 t/\hbar} (i\hbar \partial_t - \hat{H}_0) |\psi(t)\rangle_S \\
  &= e^{i\hat{H}_0 t/\hbar} (\hat{H} - \hat{H}_0) |\psi(t)\rangle_S \\
  &= e^{i\hat{H}_0 t/\hbar} V(t) e^{-i\hat{H}_0 t/\hbar} V_I(t) |\psi(t)\rangle_I \\
\end{align*}
\]

We therefore have that

\[
\begin{align*}
  i\hbar \partial_t |\psi(t)\rangle_I &= V_I(t) |\psi(t)\rangle_I, \\
  V_I(t) &= e^{i\hat{H}_0 t/\hbar} V(t) e^{-i\hat{H}_0 t/\hbar}
\end{align*}
\]
\[ i\hbar \partial_t \psi(t) \|_1 = V_1(t) \psi(t) \|_1, \quad V_1(t) = e^{i\hat{H}_0 t/\hbar} V(t) e^{-i\hat{H}_0 t/\hbar} \]

- Then, if we form eigenfunction expansion, \[ \psi(t) \|_1 = \sum_n c_n(t) \|_n, \] where \[ \hat{H}_0 \|_n = E_n \|_n, \]

\[ i\hbar \partial_t \sum_n c_n(t) \|_n = e^{i\hat{H}_0 t/\hbar} V(t) e^{-i\hat{H}_0 t/\hbar} \sum_n c_n(t) \|_n \]

\[ i\hbar \sum_n \dot{c}_n(t) \|_n = \sum_n c_n(t) e^{i\hat{H}_0 t/\hbar} V(t) \frac{e^{-i\hat{H}_0 t/\hbar} \|_n}{e^{-iE_n t/\hbar} \|_n} \]

- If we now contract with a general state \[ \|_m \]

\[ \sum_n \dot{c}_n(t) \langle m \|_n = \sum_n c_n(t) \langle m e^{i\hat{H}_0 t/\hbar} V(t) e^{-iE_n t/\hbar} \|_n \]

\[ i\hbar \dot{c}_m(t) = \sum_n \langle m \| V(t) \|_n e^{i(E_m - E_n) t/\hbar} c_n(t) \]
Time-dependent potentials: general formalism

\[ i\hbar \partial_t |\psi(t)\rangle_I = V_I(t)|\psi(t)\rangle_I, \quad V_I(t) = e^{i\hat{H}_0 t/\hbar} V(t) e^{-i\hat{H}_0 t/\hbar} \]

- Then, if we form eigenfunction expansion, \(|\psi(t)\rangle_I = \sum_n c_n(t) |n\rangle\), where \(\hat{H}_0 |n\rangle = E_n |n\rangle\),

\[
i\hbar \partial_t \sum_n c_n(t) |n\rangle = e^{i\hat{H}_0 t/\hbar} V(t) e^{-i\hat{H}_0 t/\hbar} \sum_n c_n(t) |n\rangle
\]

\[
i\hbar \sum_n \dot{c}_n(t) |n\rangle = \sum_n c_n(t) e^{i\hat{H}_0 t/\hbar} V(t) \left( e^{-i\hat{H}_0 t/\hbar} |n\rangle \right) e^{-iE_n t/\hbar} |n\rangle
\]

- If we now contract with a general state \(|m\rangle\)

\[
\sum_n \dot{c}_n(t) \langle m | n \rangle = \sum_n c_n(t) \langle m | e^{i\hat{H}_0 t/\hbar} V(t) e^{-iE_n t/\hbar} | n \rangle
\]

\[
i\hbar \dot{c}_m(t) = \sum_n \langle m | V(t) | n \rangle e^{i(E_m - E_n) t/\hbar} c_n(t)
\]
Time-dependent potentials: general formalism

\[ i\hbar \dot{c}_m(t) = \sum_n \langle m|V(t)|n\rangle e^{i(E_m - E_n)t/\hbar} c_n(t) \]

So, in summary, if we expand wavefunction \(|\psi(t)\rangle_I = \sum_n c_n(t)|n\rangle\), where \(\hat{H}_0|n\rangle = E_n|n\rangle\), the Schrödinger equation,

\[ i\hbar \partial_t |\psi(t)\rangle_I = V_I(t)|\psi(t)\rangle_I \quad \text{with} \quad V_I(t) = e^{i\hat{H}_0 t/\hbar} V(t) e^{-i\hat{H}_0 t/\hbar} \]

translates to the relation,

\[ i\hbar \dot{c}_m(t) = \sum_n V_{mn}(t) e^{i\omega_{mn} t} c_n(t) \]

where \(V_{mn}(t) = \langle m|V(t)|m\rangle\) and \(\omega_{mn} = \frac{1}{\hbar}(E_m - E_n) = -\omega_{nm}\).
Consider an atom with just two available atomic levels, $|1\rangle$ and $|2\rangle$, with energies $E_1$ and $E_2$. In the eigenbasis, the time-independent Hamiltonian can be written as

$$\hat{H}_0 = E_1 |1\rangle \langle 1| + E_2 |2\rangle \langle 2| \equiv \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix}$$

Note that the two-level atom mirrors a spin 1/2 system.

If the system is driven by an electric field, $\mathcal{E}(r, t) = \mathcal{E}_0(r) \cos(\omega t)$, and the states have different parity, close to resonance, $|\omega - \omega_{21}| \ll \omega_{21}$, the effective interaction potential is given by

$$V(t) \simeq \delta e^{i\omega t} |1\rangle \langle 2| + \delta e^{-i\omega t} |2\rangle \langle 1| \equiv \delta \begin{pmatrix} 0 & e^{i\omega t} \\ e^{-i\omega t} & 0 \end{pmatrix}$$

where the matrix element, $\delta = \langle 1|\mathcal{E}|2\rangle$ is presumed real.
Example: Dynamics of a driven two-level system

\[ \hat{H}_0 = E_1 |1\rangle \langle 1| + E_2 |2\rangle \langle 2| = \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix} \]

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Example: Dynamics of a driven two-level system

\[ \hat{H}_0 + V(t) = \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix} + \delta \begin{pmatrix} 0 & e^{i\omega t} \\ e^{-i\omega t} & 0 \end{pmatrix} \]

- The electric field therefore induces transitions between the states.
- If we expand the “spinor-like” wavefunction in eigenstates of \( \hat{H}_0 \), i.e. \( |\psi(t)\rangle_1 = c_1(t)|1\rangle + c_2(t)|2\rangle \), the equation
  \[ i\hbar \dot{c}_m(t) = \sum_n V_{mn}(t)e^{i\omega_{mn}t}c_n(t) \]
  translates to the quantum dynamics
  \[ i\hbar \partial_t \mathbf{c} = \delta \begin{pmatrix} 0 & e^{i(\omega - \omega_{21})t} \\ e^{-i(\omega - \omega_{21})t} & 0 \end{pmatrix} \mathbf{c}(t), \quad \omega_{21} = \frac{1}{\hbar}(E_2 - E_1) \]
  where \( \mathbf{c}(t) = (c_1(t) \ c_2(t)) \).
Example: Dynamics of a driven two-level system

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- Expanding this equation, we find
  \[ i\hbar \dot{c}_1 = \delta e^{i(\omega - \omega_{21})t} c_2, \quad i\hbar \dot{c}_2 = \delta e^{-i(\omega - \omega_{21})t} c_1 \]
  from which we obtain an equation for \( c_2 \),
  \[ \ddot{c}_2(t) - i(\omega - \omega_{21}) \dot{c}_2(t) + \left( \frac{\delta}{\hbar} \right)^2 c_2(t) = 0 \]

- With the initial conditions, \( c_1(0) = 1 \) and \( c_2(0) = 0 \), i.e. particle starts in state \( |1\rangle \), we obtain the solution,
  \[ c_2(t) = e^{-i(\omega - \omega_{21})t/2} \sin(\Omega t) \]
  where \( \Omega = ((\delta/\hbar)^2 + (\omega - \omega_{21})^2/4)^{1/2} \) is known as Rabi frequency.
Example: Dynamics of a driven two-level system

\[ i\hbar \frac{\partial}{\partial t} c = \delta \begin{pmatrix} 0 & e^{i(\omega - \omega_{21})t} \\ e^{-i(\omega - \omega_{21})t} & 0 \end{pmatrix} c(t), \quad \omega_{21} = \frac{1}{\hbar}(E_2 - E_1) \]

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  from which we obtain an equation for \( c_2 \),
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Example: Dynamics of a driven two-level system

\[ c_2(t) = A e^{-i(\omega - \omega_{21})t/2} \sin(\Omega t), \quad \Omega = \left( \left( \frac{\delta}{\hbar} \right)^2 + \left( \frac{\omega - \omega_{21}}{2} \right)^2 \right)^{1/2} \]

- Together with \( c_1(t) = \frac{i\hbar}{\delta} e^{i(\omega - \omega_{21})t} \hat{c}_2 \), we obtain the normalization, \( A = \frac{\delta}{\sqrt{\delta + \hbar^2(\omega - \omega_{21})^2/4}} \) and

\[ |c_2(t)|^2 = \frac{\delta^2}{\delta^2 + \hbar^2(\omega - \omega_{21})^2/4} \sin^2 \Omega t, \quad |c_1(t)|^2 = 1 - |c_2(t)|^2 \]

- Periodic solution describes transfer of probability between states 1 and 2. Maximum probability of occupying state 2 is Lorentzian,

\[ |c_2(t)|^2_{\text{max}} = \frac{\delta^2}{\delta^2 + \hbar^2(\omega - \omega_{21})^2/4}, \]

taking the value of unity at resonance, \( \omega = \omega_{21} \).
Example: Dynamics of a driven two-level system

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c_2(t) = Ae^{-i(\omega-\omega_{21})t/2} \sin(\Omega t), \quad \Omega = \left( \left( \frac{\delta}{\hbar} \right)^2 + \left( \frac{\omega - \omega_{21}}{2} \right)^2 \right)^{1/2}
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It is different to prepare and analyse ideal atomic two-level system.

However, circuits made of superconducting loops provide access to “two-level” systems. These have been of great interest since they (may yet) provide a platform to develop qubit operation and quantum logic circuits.

By exciting transitions between levels using a microwave pulse, coherence of the system has been recorded through Rabi oscillations.
Rabi oscillations: persistent current qubit

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![Rabi Oscillations Graph]

- By exciting transitions between levels using a microwave pulse, coherence of the system has been recorded through Rabi oscillations.
For a general time-dependent Hamiltonian, $\hat{H} = \hat{H}_0 + V(t)$, an analytical solution is usually infeasible.

However, as for the time-independent Schrödinger equation, we can develop to a perturbative expansion (in powers of interaction):

$$\ket{\psi(t)}_I = \sum_n c_n(t) \ket{n}, \quad c_n(t) = c_n^{(0)} + c_n^{(1)}(t) + c_n^{(2)}(t) + \cdots$$

where $\hat{H}_0 \ket{n} = E_n \ket{n}$, $c_n^{(m)} \sim O(V^m)$, and $c_n^{(0)}$ represents some (time-independent) initial state of the system.

As with the Schrödinger representation, in the interaction representation, $\ket{\psi(t)}_I$ related to initial state $\ket{\psi(t_0)}_I$, at time $t_0$, through a time-evolution operator,

$$\ket{\psi(t)}_I = \hat{U}_I(t, t_0) \ket{\psi(t_0)}_I$$
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\[
|\psi(t)\rangle_I = \hat{U}_I(t, t_0)|\psi(t_0)\rangle_I
\]
Substituted into Schrödinger equation \( i\hbar \partial_t |\psi(t)\rangle_I = V_1(t)|\psi(t)\rangle_I \),

\[
i\hbar \partial_t \hat{U}_1(t, t_0)|\psi(t_0)\rangle_I = V_1(t)\hat{U}_1(t, t_0)|\psi(t_0)\rangle_I
\]

Since this is true for any initial state \( |\psi(t_0)\rangle_I \), we must have

\[
i\hbar \partial_t \hat{U}_1(t, t_0) = V_1(t)\hat{U}_1(t, t_0)
\]

with the boundary condition \( U_1(t_0, t_0) = \mathbb{I} \).

Integrating \( t_0 \) to \( t \), \( i\hbar \int_{t_0}^{t} dt' \partial_{t'} \hat{U}_1(t', t_0) = i\hbar (\hat{U}_1(t, t_0) - \mathbb{I}) \), i.e.

\[
\hat{U}_1(t, t_0) = \mathbb{I} - i \frac{\hbar}{\hbar} \int_{t_0}^{t} dt' V_1(t') \hat{U}_1(t', t_0)
\]

provides self-consistent equation for \( U_1(t, t_0) \).
Time-dependent perturbation theory

\[ |\psi(t)\rangle_I = \hat{U}_I(t, t_0) |\psi(t_0)\rangle_I \]

- Substituted into Schrödinger equation \( i\hbar \partial_t |\psi(t)\rangle_I = V_1(t) |\psi(t)\rangle_I \),

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\[ i\hbar \partial_t \hat{U}_I(t, t_0) = V_1(t) \hat{U}_I(t, t_0) \]

with the boundary condition \( U_1(t_0, t_0) = I \).

- Integrating \( t_0 \) to \( t \), \( i\hbar \int_{t_0}^{t} dt' \partial_{t'} \hat{U}_I(t', t_0) = i\hbar (\hat{U}_I(t, t_0) - I) \), i.e.

\[ \hat{U}_I(t, t_0) = I - \frac{i}{\hbar} \int_{t_0}^{t} dt' V_1(t') \hat{U}_I(t', t_0) \]

provides self-consistent equation for \( U_1(t, t_0) \),
Time-dependent perturbation theory

\begin{align*}
|\psi(t)\rangle_I &= \hat{U}_I(t, t_0)|\psi(t_0)\rangle_I
\end{align*}

- Substituted into Schrödinger equation \( i\hbar \partial_t |\psi(t)\rangle_I = V_I(t) |\psi(t)\rangle_I \),

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 i\hbar \partial_t \hat{U}_I(t, t_0)|\psi(t_0)\rangle_I &= V_I(t) \hat{U}_I(t, t_0)|\psi(t_0)\rangle_I
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 \hat{U}_I(t, t_0) &= \mathbb{I} - \frac{i}{\hbar} \int_{t_0}^{t} dt' V_I(t') \hat{U}_I(t', t_0)
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provides self-consistent equation for \( U_I(t, t_0) \),
Time-dependent perturbation theory

\[ \hat{U}_1(t, t_0) = \mathbb{I} - \frac{i}{\hbar} \int_{t_0}^{t} dt' V_1(t') \hat{U}_1(t', t_0) \]

- If we substitute \( \hat{U}_1(t', t_0) \) on right hand side,

\[ \hat{U}_1(t, t_0) = \mathbb{I} - \frac{i}{\hbar} \int_{t_0}^{t} dt' V_1(t') + \left( -\frac{i}{\hbar} \right)^2 \int_{t_0}^{t} dt' V_1(t') \int_{t_0}^{t'} dt'' V_1(t'') \hat{U}_1(t'', t_0) \]

- Iterating this procedure,

\[ \hat{U}_1(t, t_0) = \sum_{n=0}^{\infty} \left( -\frac{i}{\hbar} \right)^n \int_{t_0}^{t} dt_1 \cdots \int_{t_0}^{t_{n-1}} dt_n V_1(t_1) V_1(t_2) \cdots V_1(t_n) \]

where term \( n = 0 \) translates to \( \mathbb{I} \).
Time-dependent perturbation theory

\[ \hat{U}_I(t, t_0) = I - \frac{i}{\hbar} \int_{t_0}^{t} dt' V_1(t') \left( I - \frac{i}{\hbar} \int_{t_0}^{t'} dt'' V_1(t'') \hat{U}_I(t'', t_0) \right) \]

If we substitute \( \hat{U}_I(t', t_0) \) on right hand side,

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Iterating this procedure,

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where term \( n = 0 \) translates to \( I \).
If we substitute $\hat{U}_1(t', t_0)$ on right hand side,

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\hat{U}_1(t, t_0) = \mathbb{I} - \frac{i}{\hbar} \int_{t_0}^{t} dt' V_1(t') \hat{U}_1(t', t_0)
$$

Iterating this procedure,

$$
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$$

$$
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$$

where term $n = 0$ translates to $\mathbb{I}$. 
Time-dependent perturbation theory

\[ \hat{U}_1(t, t_0) = \sum_{n=0}^{\infty} \left( -\frac{i}{\hbar} \right)^n \int_{t_0}^{t_1} dt_1 \cdots \int_{t_0}^{t_{n-1}} dt_n V_1(t_1) V_1(t_2) \cdots V_1(t_n) \]

**Remark:** Since operators \( V_1(t) \) appear as a time-ordered sequence, with

\[ t_0 \leq t_n \leq t_{n-1} \leq \cdots \leq t_1 \leq t \]

this expression is sometimes written as

\[ \hat{U}_1(t, t_0) = T \left[ e^{-\frac{i}{\hbar} \int_{t_0}^{t} dt' V_1(t')} \right] \]

where “T” denotes the time-ordering operator and is understood as the identity above.

**Note that,** for \( V \) independent of \( t \), \( \hat{U}_1(t, t_0) = e^{-\frac{i}{\hbar} Vt} \) reminiscent of the usual time-evolution operator for time-independent \( \hat{H} \).
Time-dependent perturbation theory

\[ \hat{U}_I(t, t_0) = \sum_{n=0}^{\infty} \left(-\frac{i}{\hbar}\right)^n \int_{t_0}^{t_1} dt_1 \cdots \int_{t_0}^{t_{n-1}} dt_n V_1(t_1) V_1(t_2) \cdots V_1(t_n) \]

- If a system is prepared in an initial state, \(|i\rangle\) at time \(t = t_0\), at a subsequent time, \(t\), the system will be in a final state, \(\hat{U}_I(t, t_0)|i\rangle\). Using the resolution of identity, \(\sum_n |n\rangle\langle n| = \mathbb{I}\), we therefore have

\[ \hat{U}_I(t, t_0)|i\rangle = \sum_n |n\rangle \left( \sum_n \langle n| \hat{U}_I(t, t_0) |i\rangle \right) \]

- From relation above, the coefficients in the expansion given by

\[ c_n(t) = \delta_{ni} - \frac{i}{\hbar} \int_{t_0}^{t} dt' \langle n| V_1(t') |i\rangle \]

\[ -\frac{1}{\hbar^2} \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' \langle n| V_1(t') V_1(t'') |i\rangle + \cdots \]
Time-dependent perturbation theory

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Time-dependent perturbation theory

\[ c_n(t) = \delta_{ni} - \frac{i}{\hbar} \int_{t_0}^{t} dt' \langle n | V_1(t') | i \rangle \]
\[ -\frac{1}{\hbar^2} \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' \sum_m \langle n | V_1(t') | m \rangle \langle m | V_1(t'') | i \rangle + \cdots \]

Recalling the definition, \( V_1(t) = e^{i\hat{H}_0 t/\hbar} V(t) e^{-i\hat{H}_0 t/\hbar} \), the matrix elements entering the coefficients are then given by

\[ \langle n | V_1(t) | m \rangle = \langle n | e^{i\hat{H}_0 t/\hbar} V(t) e^{-i\hat{H}_0 t/\hbar} | m \rangle \]
\[ = \langle n | V(t) | m \rangle \exp \left[ \frac{i}{\hbar} \left( E_n - E_m \right) \right] \]
\[ V_{nm} e^{i\omega_{nm} t} \]

where \( V_{nm}(t) = \langle n | V(t) | m \rangle \) denote matrix elements between the basis states of \( \hat{H}_0 \) on the perturbation, and \( \omega_{nm} = (E_n - E_m)/\hbar \).
\[ c_n(t) = \delta_{ni} - \frac{i}{\hbar} \int_{t_0}^{t} dt' \langle n | V_1(t') | i \rangle \]
\[ - \frac{1}{\hbar^2} \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' \sum_{m} \langle n | V_1(t') | m \rangle \langle m | V_1(t'') | i \rangle + \cdots \]

Therefore, using the relation, \( \langle n | V_1(t) | m \rangle = \langle n | V(t) | m \rangle e^{i\omega_{nm}t} \),

\[
c_n^{(1)}(t) = -\frac{i}{\hbar} \int_{t_0}^{t} dt' e^{i\omega_{ni}t'} V_{ni}(t')
\]
\[
c_n^{(2)}(t) = -\frac{1}{\hbar^2} \sum_{m} \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' e^{i\omega_{nm}t'+i\omega_{mi}t''} V_{nm}(t') V_{mi}(t'')
\]

As a result, we obtain transition probability \( |i \rangle \rightarrow | n \neq i \rangle \),

\[ P_{i \rightarrow n}(t) = |c_n(t)|^2 = |c_n^{(1)} + c_n^{(2)} + \cdots |^2 \]
Example: Kicked oscillator

Suppose quantum harmonic oscillator, \( \hat{H} = \hbar \omega (a^{\dagger} a + 1/2) \), prepared in ground state \( |0\rangle \) at time \( t = -\infty \). If it is perturbed by weak (transient) electric field,

\[
V(t) = -eE x e^{-t^2/\tau^2}
\]

what is probability of finding it in first excited state, \( |1\rangle \), at \( t = +\infty \)?

Working to first order in \( V \), \( P_{0\rightarrow 1} \approx |c_1^{(1)}|^2 \) where

\[
c_1^{(1)}(t) = -\frac{i}{\hbar} \int_{t_0}^{t} dt' e^{i\omega_{10}t'} V_{10}(t')
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with \( V_{10}(t') = -eE \langle 1 | x | 0 \rangle e^{-t'^2/\tau^2} \) and \( \omega_{10} = \omega \)
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with $V_{10}(t') = -e\mathcal{E}\langle 1|x|0\rangle e^{-t'^2/\tau^2}$ and $\omega_{10} = \omega$
Example: Kicked oscillator

\[ c^{(1)}_1(t) = -\frac{i}{\hbar} \int_{t_0}^{t} dt' e^{i\omega t'} V_{10}(t'), \quad V_{10}(t') = -e\mathcal{E}\langle 1|x|0 \rangle e^{-t'^2/\tau^2} \]

- Using the ladder operator formalism, with \( |1\rangle = a^\dagger |0\rangle \) and

\[ x = \sqrt{\frac{\hbar}{2m\omega}} (a + a^\dagger), \quad \langle 1|x|0 \rangle = \sqrt{\frac{\hbar}{2m\omega}} \langle 0|a(a + a^\dagger)|0 \rangle = \sqrt{\frac{\hbar}{2m\omega}} \]

- With \( \int_{t_0=-\infty}^{t \to \infty} dt' e^{i\omega t'} e^{-t'^2/\tau^2} = \sqrt{\pi \tau} \exp \left[-\frac{1}{4} \omega^2 \tau^2 \right] \),

\[ c^{(1)}_1(t \to \infty) = i\mathcal{E} \tau \sqrt{\frac{\pi}{2m\hbar\omega}} e^{-\omega^2 \tau^2 / 4} \]

- Transition probability,

\[ P_{0 \to 1} \approx |c^{(1)}_1(t)|^2 = (e\mathcal{E} \tau)^2 \left( \frac{\pi}{2m\hbar \omega} \right) e^{-\omega^2 \tau^2 / 2} \]

Note that \( P_{0 \to 1} \) is maximal for \( \tau \sim 1/\omega \).
Example: Kicked oscillator

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Note that \( P_{0 \to 1} \) is maximal for \( \tau \sim 1/\omega \).
“Sudden” perturbation – quantum quench

- Suppose there is a switch from $\hat{H}_0$ to $\hat{H}_0'$ in a time shorter than any other characteristic scale – perturbation theory is irrelevant:

- If system is initially in eigenstate $|n\rangle$ of $\hat{H}_0$, time evolution after switch will just follow that of $\hat{H}_0'$, i.e. simply expand initial state as a sum over eigenstates of $\hat{H}_0'$,

$$|n\rangle = \sum_{n'} |n'\rangle\langle n'|n\rangle, \quad |n(t)\rangle = \sum_{n'} e^{-iE_{n'}t/\hbar} |n'\rangle\langle n'|n\rangle$$

- “Non-trivial” part of the problem lies in establishing that the change is sudden enough.

- This is achieved by estimating the actual time taken for the Hamiltonian to change, and the periods of motion associated with the state $|n\rangle$ and with its transitions to neighbouring states.
“Sudden” perturbation – quantum quench

Suppose there is a switch from $\hat{H}_0$ to $\hat{H}'_0$ in a time shorter than any other characteristic scale – perturbation theory is irrelevant:

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i.e. simply expand initial state as a sum over eigenstates of $\hat{H}'_0$,

$$|n\rangle = \sum_{n'} |n'\rangle\langle n'|n\rangle, \quad |n(t)\rangle = \sum_{n'} e^{-iE_{n'}t/\hbar} |n'\rangle\langle n'|n\rangle$$

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This is achieved by estimating the actual time taken for the Hamiltonian to change, and the periods of motion associated with the state $|n\rangle$ and with its transitions to neighbouring states.
Harmonic perturbations: Fermi’s Golden Rule

Consider system prepared in initial state $|i\rangle$ and perturbed by a periodic harmonic potential $V(t) = V e^{-i\omega t}$ which is abruptly switched on at time $t = 0$.

e.g. atom perturbed by an external oscillating electric field.

What is the probability that, at some later time $t$, the system is in state $|f\rangle$?

To first order in perturbation theory,

$$c_t^{(1)}(t) = -\frac{i}{\hbar} \int_{t_0}^{t} dt' e^{i\omega ft'} V_{fi}(t')$$

i.e. probability of effecting transition after a time $t$,

$$P_{i\rightarrow f}(t) \simeq |c_t^{(1)}(t)|^2 = \left| -\frac{i}{\hbar} \langle f| V |i\rangle e^{i(\omega f - \omega)t/2} \frac{\sin((\omega fi - \omega)t/2)}{(\omega fi - \omega)/2} \right|^2$$
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Consider a system prepared in the initial state $|i\rangle$ and perturbed by a periodic harmonic potential $V(t) = Ve^{-i\omega t}$ which is abruptly switched on at time $t = 0$.

For example, an atom perturbed by an external oscillating electric field.

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i.e. probability of effecting transition after a time $t$,

$$P_{i\rightarrow f}(t) \propto |c_f^{(1)}(t)|^2 = \left| -\frac{i}{\hbar} \langle f|V|i\rangle e^{i(\omega_{fi} - \omega)t/2} \frac{\sin((\omega_{fi} - \omega)t/2)}{(\omega_{fi} - \omega)/2} \right|^2$$
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Harmonic perturbations: Fermi’s Golden Rule

\[ P_{i \to f}(t) \sim \frac{1}{\hbar^2} |\langle f | V | i \rangle|^2 \left( \frac{\sin((\omega_f - \omega)t/2)}{(\omega_f - \omega)/2} \right)^2 \]

- Setting \( \alpha = (\omega_f - \omega)/2 \), probability \( \sim \sin^2(\alpha t)/\alpha^2 \) with a peak at \( \alpha = 0 \) – maximum value \( t^2 \), width \( O(1/t) \sim \) total weight \( O(t) \).

- For large \( t \), \( \lim_{t \to \infty} \frac{1}{t} \left( \frac{\sin(\alpha t)}{\alpha} \right)^2 = \pi \delta(\alpha) = 2\pi \delta(2\alpha) \)

- Fermi’s Golden rule: transition rate,

\[ R_{i \to f}(t) = \lim_{t \to \infty} \frac{P_{i \to f}(t)}{t} = \frac{2\pi}{\hbar^2} |\langle f | V | i \rangle|^2 \delta(\omega_f - \omega) \]
Harmonic perturbations: Fermi’s Golden Rule

\[ P_{i \rightarrow f}(t) \approx \frac{1}{\hbar^2} |\langle f | V | i \rangle|^2 \left( \frac{\sin((\omega_f - \omega)t/2)}{(\omega_f - \omega)/2} \right)^2 \]

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- **Fermi’s Golden rule**: transition rate,

\[ R_{i \rightarrow f}(t) = \lim_{t \to \infty} \frac{P_{i \rightarrow f}(t)}{t} = \frac{2\pi}{\hbar^2} |\langle f | V | i \rangle|^2 \delta(\omega_f - \omega) \]
Harmonic perturbations: Fermi’s Golden Rule

\[ R_{i \rightarrow f}(t) = \frac{2\pi}{\hbar^2} |\langle f | V | i \rangle|^2 \delta(\omega_{fi} - \omega) \]

- This result shows that, for a transition to occur, to satisfy energy conservation we must have:
  - (a) final states exist over a continuous energy range to match \( \Delta E = \hbar \omega \) for fixed perturbation frequency \( \omega \), or
  - (b) perturbation must cover sufficiently wide spectrum of frequency so that a discrete transition with \( \Delta E = \hbar \omega \) is possible.

- For any two discrete pair of states \( |i\rangle \) and \( |f\rangle \), since \( |V_{fi}|^2 = |V_{if}|^2 \), we have \( P_{i \rightarrow f} = P_{f \rightarrow i} \)
  
  statement of detailed balance.
Harmonic perturbations: second order transitions

- Although first order perturbation theory often sufficient, sometimes $\langle \psi | V | \phi \rangle = 0$ by symmetry (e.g. parity, selection rules, etc.). In such cases, transition may be accomplished by indirect route through other non-zero matrix elements.

- At second order of perturbation theory,

$$c_f^{(2)}(t) = -\frac{1}{\hbar^2} \sum_m \int_{t_0}^{t} dt' \int_{t_0}^{t} dt'' e^{i\omega_m t' + i\omega_i t''} V_f m(t') V_m i(t'')$$

- If harmonic potential perturbation is gradually switched on, $V(t) = e^{\varepsilon t} V e^{-i\omega t}$, $\varepsilon \to 0$, with the initial time $t_0 \to -\infty$,

$$c_f^{(2)}(t) = -\frac{1}{\hbar^2} \sum_m \langle \psi | V | m \rangle \langle m | V | \phi \rangle$$

$$\times \int_{-\infty}^{t} dt' \int_{-\infty}^{t} dt'' e^{i(\omega_m - \omega - i\varepsilon) t'} e^{i(\omega_i - \omega - i\varepsilon) t''}$$
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\[
c_f^{(2)}(t) = -\frac{1}{\hbar^2} \sum_m \langle f | V | m \rangle \langle m | V | i \rangle \times \int_{-\infty}^{t} dt' \int_{-\infty}^{t'} dt'' e^{i(\omega mt - \omega t - i\varepsilon t')} e^{i(\omega mi - \omega t - i\varepsilon t'')}
\]
Harmonic perturbations: second-order transitions

1. From time integral,

\[ c_n^{(2)} = -\frac{1}{\hbar^2} e^{i(\omega_f - 2\omega)t} e^{2\varepsilon t} \sum_m \frac{\langle f|V|m\rangle\langle m|V|i \rangle}{\omega_m - \omega - i\varepsilon} \]

2. Leads to transition rate (\(\varepsilon \to 0\)):

\[ \frac{d}{dt} |c_n^{(2)}(t)|^2 = \frac{2\pi}{\hbar^4} \sum_m \frac{\langle f|V|m\rangle\langle m|V|i \rangle}{\omega_m - \omega - i\varepsilon} \delta(\omega_f - 2\omega) \]

This translates to a transition in which system gains energy \(2\hbar\omega\) from harmonic perturbation, i.e. two “photons” are absorbed – Physically, first photon takes effect virtual transition to short-lived intermediate state with energy \(\omega_m\).

If an atom in an arbitrary state is exposed to monochromatic light, other second order processes in which two photons are emitted, or one is absorbed and one emitted are also possible.
Harmonic perturbations: second-order transitions

From time integral,

\[ c^{(2)}_n = -\frac{1}{\hbar^2} e^{i(\omega_f - 2\omega)t} \frac{e^{2\epsilon t}}{\omega_f - 2\omega - 2i\epsilon} \sum_m \frac{\langle f | V | m \rangle \langle m | V | i \rangle}{\omega_m - \omega - i\epsilon} \]

Leads to transition rate (\(\epsilon \to 0\)):

\[ \frac{d}{dt} |c^{(2)}_n(t)|^2 = \frac{2\pi}{\hbar^4} \left| \sum_m \frac{\langle f | V | m \rangle \langle m | V | i \rangle}{\omega_m - \omega - i\epsilon} \right|^2 \delta(\omega_f - 2\omega) \]

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Leads to transition rate \( (\epsilon \rightarrow 0) \):

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For a general time-dependent Hamiltonian, $\hat{H} = \hat{H}_0 + V(t)$, in which all time-dependence containing in potential $V(t)$, the wavefunction can be expressed in the interaction representation,

$$|\psi(t)\rangle_I = e^{i\hat{H}_0 t/\hbar} |\psi(t)\rangle_S, \quad |\psi(0)\rangle_I = |\psi(0)\rangle_S$$

In this representation, the time-dependent Schrödinger equation takes the form,

$$i\hbar \partial_t |\psi(t)\rangle_I = V_I(t) |\psi(t)\rangle_I, \quad V_I(t) = e^{i\hat{H}_0 t/\hbar} V(t) e^{-i\hat{H}_0 t/\hbar}$$

If we expand $|\psi(t)\rangle_I = \sum_n c_n(t) |n\rangle$ in basis of time-independent Hamiltonian, $\hat{H}_0 |n\rangle = E_n |n\rangle$, the Schrödinger equation translates to

$$i\hbar \dot{c}_m(t) = \sum_n V_{mn}(t) e^{i\omega_{mn} t} c_n(t)$$

where $V_{mn}(t) = \langle m|V(t)|m\rangle$ and $\omega_{mn} = \frac{1}{\hbar} (E_m - E_n) = -\omega_{nm}$. 
For a general time-dependent Hamiltonian, $\hat{H} = \hat{H}_0 + V(t)$, in which all time-dependence containing in potential $V(t)$, the wavefunction can be expressed in the interaction representation,

$$|\psi(t)\rangle_I = e^{i\hat{H}_0 t/\hbar} |\psi(t)\rangle_S, \quad |\psi(0)\rangle_I = |\psi(0)\rangle_S$$

In this representation, the time-dependent Schrödinger equation takes the form,

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Time-dependent perturbation theory: summary

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For a general time-dependent potential, $V(t)$, the wavefunction can be expanded as a power series in the interaction,

$$|\psi(t)\rangle_I = \sum_n c_n(t)|n\rangle, \quad c_n(t) = c_n^{(0)} + c_n^{(1)}(t) + c_n^{(2)}(t) + \cdots$$

The coefficients can be expressed as matrix elements of the time-evolution operator, $c_n(t) = \langle n|\hat{U}_I(t, t_0)|i\rangle$, where

$$\hat{U}_I(t, t_0) = \sum_{n=0}^{\infty} \left(-\frac{i}{\hbar}\right)^n \int_{t_0}^{t} dt_1 \cdots \int_{t_0}^{t_{n-1}} dt_n V_1(t_1)V_1(t_2)\cdots V_1(t_n)$$

From first two terms in the series, we have

$$c_n^{(1)}(t) = -\frac{i}{\hbar} \int_{t_0}^{t} dt' e^{i\omega_{ni}t'} V_{ni}(t')$$

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$$R_{i \rightarrow f}(t) = \lim_{t \rightarrow \infty} \frac{P_{i \rightarrow f}(t)}{t} = \frac{2\pi}{\hbar^2} |\langle f | V | i \rangle|^2 \delta(\omega_f - \omega)$$

Fermi’s Golden rule.

If this term vanishes by symmetry, transitions can be effected by second and higher order processes through intermediate states.

In the next lecture, we will apply these ideas to the consideration of radiative transitions in atoms.
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