Quantum Mechanics II

Time-Dependent Physics

Time-Dependent Perturbation Theory; Harmonic Perturbations and Fermi's Rule; Radiative Perturbation

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Time-Dependent Phenomena

Program

- Spin Dynamics
  - Interaction picture; spin precession, resonance
- Exponential and Non-Exponential Decay
  - Decay probability; Quantum Zeno and anti-Zeno paradoxes
- Energy-Time Indeterminacy
  - Indeterminacy; Clock operators, characteristic times
- Quantum Beats
  - Three-state configuration, transitions; neutrino oscillations
- **Time-Dependent Perturbation Theory**
  - **Iterative master equation; 1st order transition; Fermi's golden rule**
- **Radiation and Adiabatic Approximation**
  - **Electric dipole app.; Emission/absorption; Adiabatic app.**

Time-Dependent Phenomena

Time-Dependent Perturbation Theory

- Split the Hamiltonian in the Schrödinger equation

$$i\hbar\frac{\mathrm{d}|\Psi\rangle}{\mathrm{d}t} = \left[\,\widehat{H}_0 + \lambda\widehat{H}_1(t)\,\right]|\Psi\rangle$$

- into the well-known part $\hat{H}_0$, for which

$$\widehat{H}_0\,|n\rangle = \varepsilon_n\,|n\rangle \quad \text{is well-known}$$

- and $\hat{H}_1(t)$, the (interaction) "perturbation,"
- and where λ will again serve as a bookkeeping device.
- As in stationary state perturbation theory
  - Assume that the perturbation is weak enough, so that its effects may be described in terms of a (formal) power-series in λ.
  - The basis $|\,n\,\rangle$ is complete, and so may be used to expand $|\,\Psi\rangle$

$$|\Psi\rangle := |\Psi(t)\rangle = \sum_n \boxed{a_n(t)}\, e^{-i\varepsilon_n t/\hbar}\,|n\rangle$$

focus!

Time-Dependent Phenomena

Time-Dependent Perturbation Theory

$$i\hbar\frac{\mathrm{d}|\Psi\rangle}{\mathrm{d}t} = \left[\,\widehat{H}_0 + \lambda\widehat{H}_1(t)\,\right]|\Psi\rangle$$

- Substituting the expansion,

$$|\Psi\rangle := |\Psi(t)\rangle = \sum_n a_n(t)\,e^{-i\varepsilon_n t/\hbar}\,|n\rangle$$

- …we obtain:

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\Big(\sum_n a_n(t)\,e^{-i\varepsilon_n t/\hbar}\,|n\rangle\Big) = \left[\,\widehat{H}_0 + \lambda\widehat{H}_1(t)\,\right]\Big(\sum_n a_n(t)\,e^{-i\varepsilon_n t/\hbar}\,|n\rangle\Big)$$

$$\sum_n \Big(i\hbar\,\dot{a}_n(t) + \varepsilon_n\,a_n(t)\Big)e^{-i\varepsilon_n t/\hbar}\,|n\rangle = \sum_n \Big(\varepsilon_n + \lambda\widehat{H}_1(t)\Big)a_n(t)e^{-i\varepsilon_n t/\hbar}\,|n\rangle$$

$$i\hbar\sum_n \dot{a}_n(t)\,e^{-i\varepsilon_n t/\hbar}\,|n\rangle = \lambda\sum_n \widehat{H}_1(t)\,|n\rangle\;e^{-i\varepsilon_n t/\hbar}\,a_n(t)$$

- Now, project by applying $\langle m|$

$$i\hbar\,\dot{a}_m(t)\,e^{-i\varepsilon_m t/\hbar} = \lambda\sum_n\langle m|\widehat{H}_1(t)|n\rangle\,e^{-i\varepsilon_n t/\hbar}\,a_n(t)$$

- and, finally:

$$\dot{a}_m(t) = \frac{\lambda}{i\hbar}\sum_n\langle m|\widehat{H}_1(t)|n\rangle\,e^{i\omega_{mn}t}\,a_n(t)$$

A system of (exact!) differential equations

$$\omega_{mn} := \frac{\varepsilon_m - \varepsilon_n}{\hbar}$$

Time-Dependent Phenomena

Time-Dependent Perturbation Theory

$$\dot{a}_m(t) = \frac{\lambda}{i\hbar}\sum_n \langle m|\hat{H}_1(t)|n\rangle\, e^{i\omega_{mn}t}\, a_n(t)$$

- If the basis $|n\rangle$ is finite and small enough
- this differential system

$$\begin{bmatrix}\dot{a}_1(t)\\ \dot{a}_2(t)\\ \dot{a}_3(t)\end{bmatrix} = \frac{\lambda}{i\hbar}\begin{bmatrix}M_{11}(t) & M_{12}(t) & M_{13}(t)\\ M_{21}(t) & M_{22}(t) & M_{23}(t)\\ M_{31}(t) & M_{32}(t) & M_{33}(t)\end{bmatrix}\begin{bmatrix}a_1(t)\\ a_2(t)\\ a_3(t)\end{bmatrix}$$

- may be solved exactly.

$$M_{mn}(t) := \langle m|\hat{H}_1(t)|n\rangle e^{i\omega_{mn}t}$$

- Otherwise, expand:

$$a_n(t) = \sum_{k=0}^{\infty}\lambda^k a_n^{(k)}(t)$$

analytic in λ!

shift $k \to k-1$

$$\sum_{k=0}^{\infty}\lambda^k \dot{a}_m^{(k)}(t) = \frac{\lambda}{i\hbar}\sum_n M_{mn}(t)\sum_{k=0}^{\infty}\lambda^k a_n^{(k)}(t)$$

$$= \frac{1}{i\hbar}\sum_n M_{mn}(t)\sum_{k=1}^{\infty}\lambda^k a_n^{(k-1)}(t)$$

$$\lambda^0\underbrace{\left\{\dot{a}_m^{(0)}(t)\right\}}_{=0} + \sum_{k=1}^{\infty}\lambda^k\underbrace{\left\{\dot{a}_m^{(k)}(t) - \frac{1}{i\hbar}\sum_n M_{mn}(t)a_n^{(k-1)}(t)\right\}}_{=0} = 0$$

initial *constants* — recursion relations

Time-Dependent Phenomena

Time-Dependent Perturbation Theory

$$\dot{a}_m(t) = \frac{\lambda}{i\hbar}\sum_n \langle m|\widehat{H}_1(t)|n\rangle\, e^{i\omega_{mn}t}\, a_n(t)$$

- This differential system is thus equivalent to

$$a_n^{(0)} = const. \qquad \dot{a}_n^{(k)}(t) = \frac{1}{i\hbar}\sum_n M_{mn}(t)a_n^{(k-1)}(t),\ \ k = 1,2,3\ldots$$

initial constants — recursion relations (not differential equations!)

$$a_m^{(k)}(T) = \frac{1}{i\hbar}\sum_n \int_0^T \mathrm{d}t\ \langle m|\widehat{H}_1(t)|n\rangle e^{i\omega_{mn}t}\, a_n^{(k-1)}(t),\ \ k = 1,2,3\ldots$$

- This is an iterative solution: starting with the initial constants
- …compute the k^{th} iteration (approximation) of the amplitudes
- A typical set-up: $a_i^{(0)} = 1,\ \ a_n^{(0)} = 0\ \ n \neq i; \quad |\Psi(0)\rangle = |i\rangle\,.$
- Then,

$$a_f^{(1)}(T) = \frac{1}{i\hbar}\int_0^T \mathrm{d}t\ \langle f|\widehat{H}_1(t)|i\rangle\, e^{i\omega_{fi}t}$$

- and

$$\mathrm{Prob}(f_{(t=T)}|i_{(t=0)}) = |a_f^{(1)}(T)|^2$$

is the "transition probability," to first order in perturbation theory after finite (long) time T.

QM II

Time-Dependent Phenomena

Time-Dependent Perturbation Theory

- Caution:
- After a finite time T, the system has not *transitioned (turned)*
  - from $|\Psi(0)\rangle = |i\rangle$ into $|\Psi(T)\rangle = e^{-i\varepsilon_f t/\hbar}|f\rangle$!!
  - Rather, $|\Psi(0)\rangle = |i\rangle \rightarrow \left(a_i(T)\, e^{-i\varepsilon_i t/\hbar}|i\rangle + a_f(T)\, e^{-i\varepsilon_f t/\hbar}|f\rangle + \dots\right)$
  - …a non-stationary coherent linear combination of $\hat{H}_0$-stationary states
- On the other hand,
  - $1 = |a_i(t)|^2 + \Sigma_{n\neq i}|a_n(t)|^2$, so that $|a_i(t)|^2 = 1 - \Sigma_{n\neq i}|a_n(t)|^2$
  - Now $a_n(t) = \mathrm{O}(\lambda)$, so $|a_n(t)|^2 = \mathrm{O}(\lambda^2)$, so $|a_i(t)|^2 = 1 - \mathrm{O}(\lambda^2)$

$$\sqrt{1-x^2} = 1 - \tfrac{1}{2}x^2 - \tfrac{1}{8}x^4 - \cdots = 1 - O(x^2)$$

  - then $|a_i(t)| = 1 - \mathrm{O}(\lambda^2)$ also, and to $\mathrm{O}(\lambda)$, only the phase of $a_i(t)$ changes
- In general,
  - if a calculation vanished to first order in perturbation theory
  - calculate to second order. **At least.**

Time-Dependent Phenomena

Harmonic Perturbations & Fermi's Rule

- Often, $\hat{H}_1(t) = \hat{A}\, e^{-i\omega t} + \hat{A}^\dagger\, e^{i\omega t}$, for $0 \le t \le T$, zero otherwise.
- Then $a_f^{(1)}(T) = \frac{1}{i\hbar}\langle f|\hat{A}|i\rangle \int_0^T \mathrm{d}t\; e^{i(\omega_{fi}-\omega)t} + \frac{1}{i\hbar}\langle f|\hat{A}^\dagger|i\rangle \int_0^T \mathrm{d}t\; e^{i(\omega_{fi}+\omega)t}$

$$= \frac{\langle f|\hat{A}|i\rangle}{\hbar}\,\frac{1-e^{i(\omega_{fi}-\omega)T}}{\omega_{fi}-\omega} + \frac{\langle f|\hat{A}^\dagger|i\rangle}{\hbar}\,\frac{1-e^{i(\omega_{fi}+\omega)T}}{\omega_{fi}+\omega}$$

absorption resonance $\varepsilon_f = \varepsilon_i + \hbar\omega$ emission resonance $\varepsilon_f = \varepsilon_i - \hbar\omega$

- Near resonance, when $T \to \infty$:

$$\left|a_f^{(1)}(T)\right|^2 = \frac{\left|\langle f|\hat{A}|i\rangle\right|^2}{\hbar^2}\,\frac{\left|1-e^{i(\omega_{fi}-\omega)T}\right|^2}{(\omega_{fi}-\omega)^2} = \frac{\left|\langle f|\hat{A}|i\rangle\right|^2}{\hbar^2}\left[\frac{\sin\left[\frac{1}{2}(\omega_{fi}-\omega)T\right]}{\frac{1}{2}(\omega_{fi}-\omega)}\right]^2$$

$$\xrightarrow{T\to\infty} \frac{\left|\langle f|\hat{A}|i\rangle\right|^2}{\hbar^2}\,2\pi\, T\,\delta(\omega_{fi}-\omega) = \frac{\left|\langle f|\hat{A}|i\rangle\right|^2}{\hbar}\,2\pi\, T\,\delta(\varepsilon_f-\varepsilon_i-\hbar\omega)$$

energy conservation law

Time-Dependent Phenomena

Harmonic Perturbations & Fermi's Rule

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- Then $a_f^{(1)}(T) = \frac{1}{i\hbar}\langle f|\hat{A}|i\rangle \int_0^T \mathrm{d}t\, e^{i(\omega_{fi}-\omega)t} + \frac{1}{i\hbar}\langle f|\hat{A}^\dagger|i\rangle \int_0^T \mathrm{d}t\, e^{i(\omega_{fi}+\omega)t}$

$$= \frac{\langle f|\hat{A}|i\rangle}{\hbar}\,\frac{1-e^{i(\omega_{fi}-\omega)T}}{\omega_{fi}-\omega} + \frac{\langle f|\hat{A}^\dagger|i\rangle}{\hbar}\,\frac{1-e^{i(\omega_{fi}+\omega)T}}{\omega_{fi}+\omega}$$

absorption resonance $\varepsilon_f = \varepsilon_i + \hbar\omega$ — emission resonance $\varepsilon_f = \varepsilon_i - \hbar\omega$

- Near resonance, when $T \to \infty$:

$$\left|a_f^{(1)}(T)\right|^2 = \frac{\left|\langle f|\hat{A}|i\rangle\right|^2}{\hbar^2}\,\frac{\left|1-e^{i(\omega_{fi}-\omega)T}\right|^2}{(\omega_{fi}-\omega)^2} = \frac{\left|\langle f|\hat{A}|i\rangle\right|^2}{\hbar^2}\left[\frac{\sin\left[\frac{1}{2}(\omega_{fi}-\omega)T\right]}{\frac{1}{2}(\omega_{fi}-\omega)}\right]^2$$

$$\xrightarrow{T\to\infty} \frac{\left|\langle f|\hat{A}|i\rangle\right|^2}{\hbar^2}2\pi\, T\,\delta(\omega_{fi}-\omega) = \frac{\left|\langle f|\hat{A}|i\rangle\right|^2}{\hbar}2\pi\, T\,\delta(\varepsilon_f-\varepsilon_i-\hbar\omega)$$

"transition rate"

$$\mathrm{d}R_{i\to f}(T) := \frac{1}{T}\left|a_f^{(1)}(T)\right|^2 \eta(\varepsilon_f)\,\mathrm{d}\varepsilon_f = \frac{2\pi}{\hbar}\left|\langle f|\hat{A}|i\rangle\right|^2\delta(\varepsilon_f-\varepsilon_i-\hbar\omega)\,\eta(\varepsilon_f)\,\mathrm{d}\varepsilon_f$$

$$R_{i\to f}(T) = \frac{2\pi}{\hbar}\left|\langle f|\hat{A}|i\rangle\right|^2\eta(\varepsilon_i+\hbar\omega)$$ Fermi's "golden" rule

Time-Dependent Phenomena

Radiative Perturbation

- Charged particle in EM field:

$$\hat{H}_0 = \frac{1}{2M}\left(\vec{\hat{P}} - \tfrac{q}{c}\vec{A}(\vec{r}\,)\right)^2 + W(\vec{r}\,) + q\,\Phi(\vec{r}\,)$$

$$= \underbrace{\frac{1}{2M}\vec{\hat{P}}\cdot\vec{\hat{P}} + W}_{\hat{H}_0} + \underbrace{\frac{q}{2Mc}\left(\vec{\hat{P}}\cdot\vec{A} + \vec{A}\cdot\vec{\hat{P}}\right) + \frac{q^2}{2Mc^2}\vec{A}\cdot\vec{A} + q\,\Phi}_{\hat{H}_1}$$

- But…

$$\vec{A} \simeq \vec{A} + \vec{\nabla}\chi(\vec{r},t)$$

$$\Phi \simeq \Phi - \frac{1}{c}\frac{\partial\chi(\vec{r},t)}{\partial t}$$

$$\Psi \simeq e^{i(q/\hbar c)\chi(\vec{r},t)}\,\Psi$$

ar bi tra ry !!

$$|\Psi(t)\rangle = \sum_n a_n(t)e^{-i\varepsilon_n t/\hbar}\,|n\rangle$$

$$\simeq \sum_n \left(e^{i(q/\hbar c)\chi(\vec{r},t)}\,a_n(t)\right)e^{-i\varepsilon_n t/\hbar}\,|n\rangle$$

$$a_m(t) \neq \sum_n \left\langle m\middle|e^{i(q/\hbar c)\chi(\vec{r},t)}\middle|n\right\rangle a_n(t)$$

gauge transformation

$$|a_m(t)|^2 \neq \left|\sum_n \langle m|e^{i(q/\hbar c)\chi(\vec{r},t)}|n\rangle\, a_n(t)\right|^2$$

Time-Dependent Phenomena

Radiative Perturbation

- No two ways about it: $|a_n(t)|^2$ is not gauge-invariant.
- Nevertheless, observables (decay rates, oscillation frequencies, …) are gauge-invariant, must be carefully defined.
- Restrict to $\hat{H}_1(t) \neq 0$ only within $0 \leq t \leq T$.
- Choose $\vec{A} = 0$ and $\Phi = -\int_C \mathrm{d}\vec{r} \cdot \vec{E}(\vec{r}, t)$ path-independent because $\vec{\nabla} \times \vec{E} = 0$
- Assume also

$$\vec{\nabla} \cdot \vec{E} \approx 0 \quad \Rightarrow \quad \Phi \approx -\vec{r} \cdot \vec{E}(\vec{0}, t) \qquad \hat{H}_1 = -q\vec{r} \cdot \vec{E}(0, t)$$

- For harmonic perturbations,

$$\hat{H}_1 = -q\vec{r} \cdot \vec{E}_0 \left(e^{i\omega t} + e^{-i\omega t}\right) = -2q\, x \left|\vec{E}_0\right| \cos(\omega t)$$

by choosing the coordinate system

- This produces

$$R_{i\to f}(T) = \tfrac{4\pi^2}{3}\left(\tfrac{q}{\hbar}\right)^2 u(\omega_{fi}) \left|\langle f|x|i\rangle\right|^2$$

EM energy density @ resonant frequency

Time-Dependent Phenomena

Radiative Perturbation

- Caution: if within $0 \le t \le T$ $\quad \Phi \approx -\vec{r}\cdot\vec{E}(\vec{0},t)$
- but vanishes before and after (abruptly)
  - then, Maxwell's Eqs. & $\quad \vec{E} = -\vec{\nabla}\Phi - \frac{1}{c}\frac{\partial\vec{A}}{\partial t} \qquad \vec{B} = \vec{\nabla}\times\vec{A}$
  - do not allow setting $\quad \vec{A} = 0$
  - Eh?
  - Well, if $\Phi = \Phi(t)$ like a step-function, so is $\vec{E}(\vec{r},t)$
  - But then, there is a $\delta(t)$-function displacement current, $\frac{\partial\vec{E}}{\partial t}$
  - …being a $\delta(t)$-function source for the magnetic field,… … … … … …
- Also, the EM radiation should also be treated QM
  - Read p. 361–363
  - Especially the "A-" and "B-coefficients": Eq. (12.78) (Albert Einstein)
  - Spontaneous emission probability *vs.* induced emission probability

Read Section 12.7

Quantum Mechanics II

Now, go forth and calculate!!

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