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Problem Sheet 3
for the tutorial on May 23rd, 2025
Quantum Mechanics II
Summer term 2025

Sheet handed out on May 13th, 2025; to be handed in on May 20th, 2025 until 2 pm

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Exercise 3.1: Time-dependent perturbation theory for harmonic oscillator [8 P.]

In the lecture we discussed periodic perturbations. As a further example we here consider a one-dimensional harmonic oscillator with mass m, charge e, and frequency ω in a time-dependent electric field

$$E(t) = \frac{A}{\tau\sqrt{\pi}} e^{-(t/\tau)^2} \cos \Omega t. \tag{1}$$

where $A \in \mathbb{R}$is a constant, $\tau > 0$ is the decay rate and $\Omega > 0$ is the field frequency.
The Hamiltonian reads

$$\hat{\mathcal{H}}_p = \hat{\mathcal{H}}_0 + \hat{\mathcal{H}}'(t) \tag{2}$$

where

$$\hat{\mathcal{H}}_0 = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 \hat{x}^2 \tag{3}$$

is the well-known harmonic oscillator Hamiltonian and the perturbation is given by

$$\hat{\mathcal{H}}'(t) = e\hat{x}E(t). \tag{4}$$

Calculate the transition probability $P_{0\to n}(t_0, t)$ from the ground state $|0\rangle$ at $t_0 \to -\infty$ to an excited state $|n\rangle$ at $t \to \infty$ in first order perturbation theory. What happens for $\tau \to 0$?

Exercise 3.2: Time evolution operator [4 + 5 P.]

a) Let

$$\mathcal{H} = \mathcal{H}_A(t) + \mathcal{H}_B(t). \tag{5}$$

Show that a time-evolution operator $\mathcal{U}(t, t')$ fulfilling

$$\mathcal{U}(t, t') = \mathcal{U}_A(t, t') - \frac{i}{\hbar} \int_{t'}^{t} dt'' \, \mathcal{U}_A(t, t'')\mathcal{H}_B(t'')\mathcal{U}(t'', t') \tag{6}$$

also satisfies the time-dependent Schrödinger equation

$$i\hbar\partial_t \mathcal{U}(t, t') = \mathcal{H}(t)\mathcal{U}(t, t') \tag{7}$$

if $\mathcal{U}_A(t,t')$ obeys its own time-dependent Schrödinger equation

$$i\hbar\partial_t\mathcal{U}_A(t,t') = \mathcal{H}_A(t)\mathcal{U}_A(t,t') \tag{8}$$

b) Show that

$$\mathcal{U}(t,t') = \mathcal{U}_A(t,t') - \frac{i}{\hbar}\int_{t'}^{t} dt''\,\mathcal{U}(t,t'')\mathcal{H}_B(t'')\mathcal{U}_A(t'',t'). \tag{9}$$

Exercise 3.3: **The interaction picture for the semi-classical Hamiltonian** [8 P.]

In this exercise we will work on the transformation to the interaction picture, which aims at obtaining an expression of the Hamiltonian with no explicit time dependence. Let us start from the expression of the total semi-classical Hamiltonian of a two level system with the ground state $|1\rangle$ and the excited state $|2\rangle$ interacting with a classical electric field,

$$H = \hbar\omega_1|1\rangle\langle 1| + \hbar\omega_2|2\rangle\langle 2| - \vec{E}\cdot\vec{d}\,|2\rangle\langle 1| - \vec{E}\cdot\vec{d}^*|1\rangle\langle 2| \tag{10}$$

with

$$\vec{E} = \vec{\varepsilon}\mathcal{E}e^{-i\omega t} + c.c. \tag{11}$$

The interaction picture is reached by separating a part of the Hamiltonian as $H_T = \hbar x|1\rangle\langle 1| + \hbar y|2\rangle\langle 2|$, with constants x and y to be determined. The interaction picture Hamiltonian is given by

$$V = U^\dagger(H - H_T)U \tag{12}$$

with the unitary transformation $U = e^{-\frac{i}{\hbar}H_T t}$. Using the rotating wave approximation, choose x and y such that V is time-independent and reaches the form

$$V = \hbar\Delta|2\rangle\langle 2| - \hbar\left(\Omega|2\rangle\langle 1| + \Omega^*|1\rangle\langle 2|\right)\,, \tag{13}$$

where Δ is the detuning $\Delta = (\omega_2 - \omega_1) - \omega$ and the Rabi frequency is given by $\Omega = \frac{\mathcal{E}\vec{\varepsilon}\cdot\vec{d}}{\hbar}$.

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$$|\psi(t)\rangle = \sum_n d_n(t) e^{-\frac{iE_n t}{\hbar}} |n\rangle$$

$$i\hbar \dot{d}_k = \sum_n d_n \langle k|H_1|n\rangle e^{\frac{i(E_k - E_n)t}{\hbar}}$$

$$H_1 = e\hat{x}E(t)$$

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}\,(a^\dagger + a)$$

$$H_1 = eE(t)\sqrt{\frac{\hbar}{2m\omega}}\,(a^\dagger + a)$$

$$\langle k|a^\dagger + a|n\rangle = \delta_{n+1,k}\sqrt{k} + \delta_{n-1,k}\sqrt{k+1}$$

$$i\hbar \dot{d}_k = \sum_n d_n e E(t)\sqrt{\frac{\hbar}{2m\omega}}\left[\delta_{n+1,k}\sqrt{k} + \delta_{n-1,k}\sqrt{k+1}\right] e^{\frac{i(E_k - E_n)t}{\hbar}}$$

$$= eE(t)\sqrt{\frac{\hbar}{2m\omega}}\left[d_{k-1}\sqrt{k}\, e^{\frac{i(E_k - E_{k-1})t}{\hbar}} + d_{k+1}\sqrt{k+1}\, e^{\frac{i(E_k - E_{k+1})t}{\hbar}}\right]$$

$$= eE(t)\sqrt{\frac{\hbar}{2m\omega}}\left[d_{k-1}\sqrt{k}\, e^{i\omega t} + d_{k+1}\sqrt{k+1}\, e^{-i\omega t}\right] \quad \text{(exact so far)}$$

Initial conditions: $d_k(-\infty) = \begin{cases} 1 & k=0 \\ 0 & \text{otherwise} \end{cases}$

1st order perturbation theory: We substitute the initial conditions (0th order) in RHS.

$\dot{d}_k = 0$ for all $k > 1$.

For $d_k = 1$

$$i\hbar \dot{d}_1 = eE(t)\sqrt{\frac{\hbar}{2m\omega}}e^{i\omega t}$$

$$= e\sqrt{\frac{\hbar}{2m\omega}}\ \frac{A}{\tau\sqrt{\pi}}\, e^{-\left(\frac{t}{\tau}\right)^2}\cos\Omega t\ e^{i\omega t}$$

$$d_1(\infty) = \frac{e}{i\hbar}\sqrt{\frac{\hbar}{2m\omega}}\ \frac{A}{\tau\sqrt{\pi}}\int_{-\infty}^{\infty} e^{-\left(\frac{t}{\tau}\right)^2} e^{i\omega t}\cos\Omega t\, dt$$

$$= \frac{e}{i\hbar}\sqrt{\frac{\hbar}{2m\omega}}\ \frac{A}{\tau\sqrt{\pi}}\ \sqrt{\pi}\,\tau\, e^{-\frac{\tau^2(\omega+\Omega)^2}{4}}$$

$$= -\frac{i}{\hbar} eA\sqrt{\frac{\hbar}{2m\omega}}\ e^{-\frac{\tau^2(\omega+\Omega)^2}{4}}$$

$$P_{0\to 1} = |d_1|^2 = \frac{1}{\hbar^2} e^2A^2\ \frac{\hbar}{2m\omega}\, e^{-\frac{\tau^2(\omega+\Omega)^2}{2}}$$

$$= \frac{e^2A^2}{2m\omega\hbar}\ e^{-\frac{\tau^2(\omega+\Omega)^2}{2}}$$

charge

2.718...

$$P_{0\to n} = \begin{cases} \frac{e^2A^2}{2m\omega\hbar}\ e^{-\frac{\tau^2(\omega+\Omega)^2}{2}} & n=1 \\ 0 & \text{otherwise} \end{cases}$$

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$$\partial_t \mathcal{U}(t,t') = \partial_t \mathcal{U}_A(t,t') - \frac{i}{\hbar}\partial_t \int_{t'}^{t} \mathcal{U}_A(t,t'')\mathcal{H}_B(t'')\mathcal{U}(t'',t')\,dt''$$

$$= \partial_t \mathcal{U}_A(t,t') - \frac{i}{\hbar}\left[\cancelto{1}{\mathcal{U}_A(t,t)}\,\mathcal{H}_B(t)\mathcal{U}(t,t')\right]$$

$$- \frac{i}{\hbar}\int_{t'}^{t}\left[\partial_t \mathcal{U}_A(t,t'')\right]\mathcal{H}_B(t'')\mathcal{U}(t'',t')\,dt''$$

$$= -\frac{i}{\hbar}\mathcal{H}_A(t)\mathcal{U}_A(t,t') - \frac{i}{\hbar}\mathcal{H}_B(t)\mathcal{U}(t,t')$$

$$- \frac{i}{\hbar}\int_{t'}^{t}\left(-\frac{i}{\hbar}\mathcal{H}_A(t)\mathcal{U}_A(t,t'')\right)\mathcal{H}_B(t'')\mathcal{U}(t'',t')\,dt''$$

$$= -\frac{i}{\hbar}\mathcal{H}_B(t)\mathcal{U}(t,t')$$

$$- \frac{i}{\hbar}\mathcal{H}_A(t)\left[\mathcal{U}_A(t,t') - \frac{i}{\hbar}\int_{t'}^{t}\mathcal{U}_A(t,t'')\mathcal{H}_B(t'')\mathcal{U}(t'',t')\,dt''\right]$$

$$= -\frac{i}{\hbar}\mathcal{H}_B(t)\mathcal{U}(t,t') - \frac{i}{\hbar}\mathcal{H}_A(t)\mathcal{U}(t,t')$$

$$= -\frac{i}{\hbar}\mathcal{H}(t)\mathcal{U}(t,t')$$

$$i\hbar\,\partial_t \mathcal{U}(t,t') = \mathcal{H}(t)\mathcal{U}(t,t')$$

b) Show that
$$\mathcal{U}(t,t') = \mathcal{U}_A(t,t') - \frac{i}{\hbar}\int_{t'}^{t} dt''\,\mathcal{U}(t,t'')\mathcal{H}_B(t'')\mathcal{U}_A(t'',t'). \tag{9}$$

Consider $\mathcal{H}_A(t) = \mathcal{H}(t) - \mathcal{H}_B(t)$

Conditions are satisfied to apply Eq. 7 to $\mathcal{H}_A(t)$

$$\mathcal{U}_A(t,t') = \mathcal{U}(t,t') - \frac{i}{\hbar}\int_{t'}^{t} \mathcal{U}(t,t'')\left[-\mathcal{H}_B(t)\right] \mathcal{U}_A(t'',t')\,dt''$$

Hence $$\mathcal{U}(t,t') = \mathcal{U}_A(t,t') - \frac{i}{\hbar}\int_{t'}^{t} \mathcal{U}(t,t'')\,\mathcal{H}_B(t)\,\mathcal{U}_A(t'',t')\,dt''$$

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$$U = e^{-\frac{iH_T t}{\hbar}} = e^{-\frac{i\hbar x t}{\hbar}}|1\rangle\langle 1| + e^{-\frac{i\hbar y t}{\hbar}}|2\rangle\langle 2|$$

$$= e^{-ixt}|1\rangle\langle 1| + e^{-iyt}|2\rangle\langle 2|$$

$$V = \left[e^{ixt}|1\rangle\langle 1| + e^{iyt}|2\rangle\langle 2|\right]\Big[\hbar(\omega_1 - x)|1\rangle\langle 1| + \hbar(\omega_2 - y)|2\rangle\langle 2|$$
$$- \vec{E}\cdot\vec{d}\,|2\rangle\langle 1| - \vec{E}\cdot\vec{d}^*|1\rangle\langle 2|\Big]\left[e^{-ixt}|1\rangle\langle 1| + e^{-iyt}|2\rangle\langle 2|\right]$$

$$= \left[e^{ixt}|1\rangle\langle 1| + e^{iyt}|2\rangle\langle 2|\right]\Big[\hbar(\omega_1 - x)e^{-ixt}|1\rangle\langle 1| - \vec{E}\cdot\vec{d}e^{-ixt}|2\rangle\langle 1|$$
$$+ \hbar(\omega_2 - y)e^{-iyt}|2\rangle\langle 2| - \vec{E}\cdot\vec{d}^*e^{-iyt}|1\rangle\langle 2|\Big]$$

$$= \hbar(\omega_1 - x)|1\rangle\langle 1| - \vec{E}\cdot\vec{d}^*e^{i(x-y)t}|1\rangle\langle 2| - \vec{E}\cdot\vec{d}\,e^{i(y-x)t}|2\rangle\langle 1|$$
$$+ \hbar(\omega_2 - y)|2\rangle\langle 2|$$

For time independence, choose $y = \omega_1 + \omega$, $x = \omega_1$. Then

$$\vec{E}\cdot\vec{d}\,e^{i(y-x)t} = \hbar\Omega$$

and

$$V = \hbar\Delta|2\rangle\langle 2| - \hbar\left(\Omega|2\rangle\langle 1| + \Omega^*|1\rangle\langle 2|\right)$$

as desired.