

Exercises on Quantum Mechanics II (TM1/TV)

Problem set 9, discussed December 16 - December 20, 2019

Exercise 53 (central tutorial)

In this exercise we will analyse another way of doing time-dependent perturbation theory, in which we will use the interaction picture. Let's consider a system with the Hamiltonian $\hat{H} = \hat{H}_0 + \hat{V}(t)$ where $\hat{V}(t)$ is small.

- (i) How is the time-evolution operator in the interaction picture defined?
 (ii) Show that the time-evolution operator in the interaction picture satisfies the integral equation

$$\hat{U}_I(t, t_i) = 1 - \frac{i}{\hbar} \int_{t_i}^t \hat{V}_I(t') \hat{U}_I(t, t_i) dt' \quad (1)$$

with initial conditions $\hat{U}_I(t_i, t_i) = \mathbb{1}$.

- (iii) Show that solving this equation iteratively, one obtains the "Dyson series":

$$\hat{U}_I(t, t_i) = \mathbb{1} - \frac{i}{\hbar} \int_{t_i}^t \hat{V}_I(t') dt' + \left(-\frac{i}{\hbar}\right)^2 \int_{t_i}^t \hat{V}_I(t_1) dt_1 \int_{t_i}^{t_1} \hat{V}_I(t_2) dt_2 + \dots \quad (2)$$

- (iv) Consider now the following situation. Suppose that for $t < t_i$ and $t > t_f$, the system is described by the free Hamiltonian which satisfies $\hat{H}_0 |\psi_n\rangle = E_n |\psi_n\rangle$, and, for $t_i < t < t_f$ the system is described by the Hamiltonian $\hat{H} = \hat{H}_0 + \hat{V}(t)$. What is the probability that if the system was initially in the state $|\psi_n\rangle$, it will be found in the state $|\psi_m\rangle$ with $m \neq n$, after a time interval $T = t_f - t_i$? *Hint:*

$$P(n \rightarrow m) = \left| \langle \psi_m | \hat{U}_I(t_f, t_i) | \psi_n \rangle \right|^2 \quad (3)$$

- (v) Let now H_0 be the Hamiltonian for a harmonic oscillator, and $\hat{V}(q, t) = V_0 \hat{q}^3 e^{-t/\tau}$ where V_0 is constant. Calculate the probability for a transition from the ground state at $t_i = 0$ to n 'th excited state for $t_f \rightarrow \infty$. *Hint: You may use the following integral*

$$\left| \int_0^\infty e^{-(\frac{1}{\tau} - inw)t} dt \right|^2 = \frac{1}{n^2 w^2 + \frac{1}{\tau^2}} \quad (4)$$

Solution

- (i) Let's remember that the operators in the interaction picture are given by

$$\hat{A}_I = e^{\frac{i}{\hbar} \hat{H}_0 t} \hat{A} e^{-\frac{i}{\hbar} \hat{H}_0 t} \quad (5)$$

Here $\hat{U}_0(t) = e^{-\frac{i}{\hbar} \hat{H}_0 t}$ is the time-evolution operator corresponding to the free part of the Hamiltonian. Then we can define the time-evolution operator (corresponding to the full Hamiltonian) in the interaction picture as

$$\hat{U}_I(t) = \hat{U}_0^\dagger(t, 0) \hat{U}(t, t_i) \hat{U}_0(t_i, 0) \quad (6)$$

- (ii) Here we can follow same procedure as in problem sheet 6. The state in the interaction picture satisfies the equation

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle_I = \hat{V}_I(t) |\psi(t)\rangle_I \quad (7)$$

If at a time t_i , state vector was given by $|\psi(t_i)\rangle$, at a later time, one can see that the state vector will be given by

$$|\psi(t)\rangle_I = \hat{U}_I(t, t_i) |\psi(t_i)\rangle_I \quad (8)$$

Substituting this in the previous relation, one obtains the equation for $\hat{U}_I(t, t_i)$:

$$i\hbar \frac{\partial}{\partial t} \hat{U}_I(t, t_i) = \hat{V}_I(t) \hat{U}_I(t, t_i) \quad (9)$$

from where the integral equation follows.

- (iii) Just solve it iteratively, same as in PS6.

- (iv) Plugging the expression for \hat{U}_I into the expression for probability, we find

$$P(n \rightarrow m) = \left| \langle \psi_m | \psi_n \rangle - \frac{i}{\hbar} \int_{t_i}^{t_f} \langle \psi_m | \hat{V}_I(t) | \psi_n \rangle dt + \dots \right|^2 \quad (10)$$

Assuming that $m \neq n$, the first term vanishes. Using that $\hat{V}_I(t) = \hat{U}_0^\dagger \hat{V} \hat{U}_0$, we obtain to the first order

$$P(n \rightarrow m) = \left| -\frac{i}{\hbar} \int_{t_i}^{t_f} \langle \psi_m | \hat{V}(t) | \psi_n \rangle e^{\frac{i}{\hbar}(E_m - E_n)t} dt \right|^2 \quad (11)$$

- (v)

$$P(0 \rightarrow n) = \frac{1}{\hbar^2} \left| \int_0^\infty dt \langle n | \hat{V}(t) | 0 \rangle e^{\frac{i}{\hbar}(E_n - E_0)t} \right|^2 = \frac{V_0^2}{\hbar^2} |\langle n | \hat{q}^3 | 0 \rangle|^2 \left| \int_0^\infty dt e^{\frac{i}{\hbar}(E_n - E_0)t} e^{-\frac{t}{\tau}} \right|^2 \quad (12)$$

For the harmonic oscillator we have $E_n = \hbar\omega(n + \frac{1}{2})$ and hence

$$e^{\frac{i}{\hbar}(E_n - E_0)t} e^{-\frac{t}{\tau}} = e^{-(\frac{1}{\tau} - in\omega)t} \quad (13)$$

Furthermore, we can express the coordinate \hat{q} in terms of creation and annihilation operators as $\hat{q} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^\dagger)$. Then we have

$$\langle n | \hat{q}^3 | 0 \rangle = \left(\frac{\hbar}{2m\omega} \right)^{\frac{3}{2}} \langle n | \hat{a}^{\dagger 3} + \hat{a}\hat{a}^{\dagger 2} + \hat{a}^\dagger | 0 \rangle \quad (14)$$

Using that $\hat{a}^\dagger | n \rangle = \sqrt{n+1} | n+1 \rangle$, and $\hat{a} | n \rangle = \sqrt{n} | n-1 \rangle$ we have

$$\langle n | \hat{q}^3 | 0 \rangle = \left(\frac{\hbar}{2m\omega} \right)^{\frac{3}{2}} (\sqrt{6}\delta_{n3} + 3\delta_{n1}) \quad (15)$$

From this we see that the only possible states where transition can take place are first and third excited state within the first order in perturbation theory. The probabilities of the transition from ground state to these states are given by

$$P(0 \rightarrow 1) = \frac{\hbar^3}{2m\omega} \frac{9V_0^2}{(\hbar\omega)^2 + \frac{\hbar^2}{\tau^2}} \quad (16)$$

$$P(0 \rightarrow 3) = \frac{\hbar^3}{2m\omega} \frac{6V_0^2}{(3\hbar\omega)^2 + \frac{\hbar^2}{\tau^2}} \quad (17)$$

Exercise 54 (central tutorial)

Let $|\phi_n\rangle$ be the eigenstates of the unperturbed Hamiltonian \hat{H}_0 which has no degenerate eigenvalues. The complete system shall be described by $\hat{H} = \hat{H}_0 + \hat{V}$. The correction to a state can generally be written as

$$|\bar{\phi}_n\rangle = |\phi_n\rangle + \sum_l c_n^l |\phi_l\rangle \quad (18)$$

Calculate c_n^l , at first order in \hat{V} .

Solution First way

We know that:

$$|\bar{\phi}_n\rangle = |\phi_n\rangle + \sum_l c_n^l |\phi_l\rangle \quad \text{and} \quad \langle \bar{\phi}^m | = \langle \phi^m | + \sum_k c_k^m \langle \phi^k | \quad (19)$$

It is not restrictive to set $c_n^n = 0$, since it is equivalent to a renormalization of the state. Furthermore from the condition of the state to be normalized we get:

$$\delta_n^m = \langle \bar{\phi}^m | \bar{\phi}_n \rangle = \delta_n^m + c_n^m + c_n^m + O(V^2) \quad (20)$$

The equation must be satisfied order by order and taking $m \neq n$, it follows that:

$$c_n^m + c_n^m = 0 \quad (21)$$

Considering again $m \neq n$ it follows that:

$$\begin{aligned} 0 &= \langle \bar{\phi}^m | \hat{U}(T) | \bar{\phi}_n \rangle = \sum_{\alpha, \beta} \langle \bar{\phi}^m | \phi_\alpha \rangle \underbrace{\langle \phi^\alpha | \hat{U}(T) | \phi_\beta \rangle}_{\lambda_{\alpha\beta}^\alpha} \langle \phi^\beta | \bar{\phi}_n \rangle = \sum_{\alpha, \beta} (\delta_\alpha^m + c_\alpha^m) \lambda_\beta^\alpha (\delta_n^\beta + c_n^\beta) = \\ &= \lambda_n^m + \sum_\alpha c_\alpha^m \lambda_n^\alpha + \sum_\beta c_n^\beta \lambda_\beta^m + O(V^2) \stackrel{(0)}{=} \lambda_n^m + \sum_\alpha c_\alpha^m \lambda_n^\alpha + \sum_\beta c_n^\beta \lambda_\beta^m + O(V^2) \end{aligned} \quad (22)$$

Recalling that

$${}^{(0)}\lambda_n^m = \delta_n^m e^{-\frac{i}{\hbar} E_n T}, \quad (23)$$

that we are considering $m \neq n$ and that this must be true order by order, it holds:

$${}^{(1)}\lambda_n^m + c_n^m e^{-\frac{i}{\hbar} E_n T} + c_n^m e^{-\frac{i}{\hbar} E_m T} = 0 \quad (24)$$

Using the condition of Equation 21, we find:

$$c_n^m = -\frac{{}^{(1)}\lambda_n^m}{e^{-\frac{i}{\hbar} E_m T} - e^{-\frac{i}{\hbar} E_n T}} \quad (25)$$

Using the result from the lecture for ${}^{(1)}\lambda_n^m$:

$${}^{(1)}\lambda_n^m = \frac{V_n^m}{E_n - E_m} (e^{-\frac{i}{\hbar} E_n T} - e^{-\frac{i}{\hbar} E_m T}) \quad m \neq n \quad (26)$$

we find

$$c_n^m = \frac{V_n^m}{E_n - E_m} \quad (27)$$

Therefore at first order the eigenstates of \hat{H} are

$$|\bar{\phi}_n\rangle = |\phi_n\rangle + \sum_l c_n^l |\phi_l\rangle = |\phi_n\rangle + \sum_{l \neq n} \frac{V_n^l}{E_n - E_l} |\phi_l\rangle \quad (28)$$

Second way

Suppose that free and perturbed Hamiltonian satisfies respectively

$$\hat{H}_0 |\phi_n\rangle = E_n |\phi_n\rangle \quad \hat{H} |\bar{\phi}_n\rangle = \bar{E}_n |\bar{\phi}_n\rangle \quad (29)$$

Let's expand the perturbed eigenvalues and eigenvectors into unperturbed values together with corrections. Then we have up to first order

$$\begin{aligned} \bar{E}_n &= E_n + E_n^{(1)} + \dots \\ |\bar{\phi}_n\rangle &= |\phi_n\rangle + |\phi_n^{(1)}\rangle + \dots \end{aligned} \quad (30)$$

Inserting this into the eigenvalue equation for the perturbed Hamiltonian we obtain

$$\begin{aligned} \hat{H}_0 |\phi_n\rangle &= E_n |\phi_n\rangle \\ \hat{H}_0 |\phi_n^{(1)}\rangle + \hat{V} |\phi_n\rangle &= E_n |\phi_n^{(1)}\rangle + E_n^{(1)} |\phi_n\rangle \end{aligned} \quad (31)$$

an so on...

Suppose we normalize $|\bar{\phi}_n\rangle$ such that $\langle \bar{\phi}_n | \phi_n \rangle = 1$. Then all products between corrections and unperturbed vector vanish for the same index n. Furthermore, since $|\phi_n\rangle$ make complete and orthonormal basis, we can expand the first correction in terms of them

$$|\phi_n^{(1)}\rangle = \sum_{m \neq n} \langle \phi^m | \phi_n^{(1)} \rangle |\phi_m\rangle \quad (32)$$

Now by comparison with (18) one can see that $\langle \phi^m | \phi_n^{(1)} \rangle = c_n^m$. We can determine this expression by multiplying second relation in (31) with $\langle \phi^m |$. Then we have

$$c_n^m = \frac{V_n^m}{E_n - E_m} \quad (33)$$

Exercise 55

The transition amplitude for the two level system is defined as in the lecture by

$$P_T(a \rightarrow b) = |\lambda_{ba}^{(1)}|^2 = \frac{1}{\hbar^2} \left| \int_0^T dt_I V_{ba}(t_I) e^{i\omega_{ba}t_I} \right|^2 \quad (34)$$

where

$$V_{ba}(t_I) = \int dq_I \psi_b^*(q_I) V(q_I, t_I) \psi_a(q_I) \quad \text{and} \quad \omega_{ba} = \frac{E_b - E_a}{\hbar} \quad (35)$$

is the matrix between the eigenstates of the energy levels. Show that

$$P_T(a \rightarrow b) = P_T(b \rightarrow a) \quad (36)$$

Solution It follows directly by switching a with b and complexly conjugating the expression.

Exercise 56

Prove that

$$\lim_{T \rightarrow \infty} \frac{\sin^2(\alpha T)}{\pi \alpha^2 T} = \delta(\alpha) \quad (37)$$

Hint: you may find useful the following result, $\int_{\mathbb{R}} dx \frac{\sin^2(x)}{x^2} = \pi$.

Solution To prove it let's take a test function $f(\alpha)$ and consider the following integral:

$$\begin{aligned} \lim_{T \rightarrow \infty} \int_{\mathbb{R}} d\alpha \frac{\sin^2(\alpha T)}{\pi \alpha^2 T} f(\alpha) &\stackrel{\alpha T = x}{=} \int_{\mathbb{R}} dx \lim_{T \rightarrow \infty} \frac{\sin^2(x)}{\pi x^2} f\left(\frac{x}{T}\right) = \frac{f(0)}{\pi} \underbrace{\int_{\mathbb{R}} dx \frac{\sin^2(x)}{x^2}}_{\pi} = \\ &= f(0) \end{aligned} \quad (38)$$

Since the δ -function is defined through $\int_{\mathbb{R}} d\alpha \delta(\alpha) f(\alpha) = f(0)$, we can conclude that:

$$\lim_{T \rightarrow \infty} \frac{\sin^2(\alpha T)}{\pi \alpha^2 T} = \delta(\alpha) \quad (39)$$

Exercise 57

Show for an isotropic stochastic electromagnetic field, that

$$\langle |\vec{E}|^2 \rangle = 3 \langle E_z^2 \rangle. \quad (40)$$

Solution The solution is presented in two ways.

The first one is more intuitive and relies on the fact that the expectation value of the square of the field in one direction must be equal, due to the spherical symmetry of the problem, to the one in any other direction, i.e. $\langle E_x^2 \rangle = \langle E_y^2 \rangle = \langle E_z^2 \rangle$. Thus,

$$\langle |\vec{E}|^2 \rangle = \langle E_x^2 \rangle + \langle E_y^2 \rangle + \langle E_z^2 \rangle = 3 \langle E_z^2 \rangle \quad (41)$$

The second way is more formal. Let's try to calculate the expectation value of $|\vec{E}|^2$ explicitly. Since the field is stochastic the system has a natural spherical symmetry and the probability distribution will be given by $\rho(\vec{x}) = \rho(|\vec{x}|)$.

$$\begin{aligned} \langle |\vec{E}|^2 \rangle &= \int_{\mathbb{R}^3} d^3x \rho(\vec{x}) |\vec{E}(\vec{x})|^2 = \int_{\mathbb{R}^3} d^3x \rho(|\vec{x}|) |\vec{E}(|\vec{x}|)|^2 = \int_0^\pi d\theta \sin(\theta) \underbrace{\int_0^{2\pi} d\phi \int_0^\infty dr r^2 \rho(r) |\vec{E}(r)|^2}_{\text{R}} = \\ &= \int_0^\pi d\theta \sin(\theta) R = 2R \end{aligned} \quad (42)$$

In the same way we can calculate the expectation value for the z-direction.

$$\begin{aligned} \langle E_z^2 \rangle &= \int_{\mathbb{R}^3} d^3x \rho(|\vec{x}|) |E_z(|\vec{x}|)|^2 = \int_{\mathbb{R}^3} d^3x \rho(|\vec{x}|) |\vec{E}(|\vec{x}|) \cdot \hat{n}_z|^2 = \int_{\mathbb{R}^3} d^3x \rho(|\vec{x}|) |\vec{E}(|\vec{x}|) \cos(\theta)|^2 = \\ &= \underbrace{\int_0^\pi d\theta \sin(\theta) \cos^2(\theta)^2}_{2/3} \underbrace{\int_0^{2\pi} d\phi \int_0^\infty dr r^2 \rho(r) |\vec{E}(r)|^2}_{\text{R}} = \frac{2}{3} R \end{aligned} \quad (43)$$

And thus,

$$\frac{\langle |\vec{E}|^2 \rangle}{\langle E_z^2 \rangle} = 3. \quad (44)$$

General information

The *lecture* takes place on:

Monday at 10:00 - 12:00 c.t. in B 052 (Theresienstraße 37)

Friday at 10:00 - 12:00 c.t. in B 052 (Theresienstraße 37)

The *central tutorial* takes place on Monday at 12:00 - 14:00 c.t. in B 139 (Theresienstraße 37)

The *webpage* for the lecture and exercises can be found at

https://www.physik.uni-muenchen.de/lehre/vorlesungen/wise_19_20/T_M1_TV_-Quantum-Mechanics-II