Quantum theory of light-matter interaction: Fundamentals

Lecture 6
Time-dependent perturbation theory

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BEFEKTETÉS A JÖVŐBE

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Introduction

The aim of the present lecture is to get acquainted with an important method, which is used in many areas of quantum mechanics in general.

It will be able to give account quantum mechanically about the dynamical response of an atom affected by a light field.

The method is called: *time-dependent perturbation theory*.

The actual application and the details of this method to describe the atomic response to the electromagnetic field will follow in the next Lecture.

Schrödinger equation

Quantum dynamics of the atom is governed by the time-dependent Schrödinger equation:

$$i\hbar \frac{\partial \left|\Psi(t)\right\rangle}{\partial t} = H \left|\Psi(t)\right\rangle . \qquad \text{(SchE)}$$

$\left|\Psi(t)\right\rangle$ is an abstract element of a Hilbert space, it gives the state of the atomic system.
H is the Hamiltonian, consisting of two terms:

$$H = \underbrace{H_0}_{\text{closed atomic system}} + \underbrace{K(t)}_{\substack{\text{time-dependent} \\ \text{interaction with the field}}}$$

H_0 is time independent. Its eigenstates $\left|u_j\right\rangle$, and the corresponding eigenvalues ε_j are assumed to be known. $K(t)$ is the *perturbation operator.*

Basis of stationary states

The eigenvalue equation of H_0 is $H_0 \left|u_j\right\rangle = \varepsilon_j \left|u_j\right\rangle$ with known ε_j and $\left|u_j\right\rangle$.
We will write for short: $H_0 \left|j\right\rangle = \varepsilon_j \left|j\right\rangle$.
The system of the stationary states $\left|j\right\rangle$ is an orthonormal set of vectors: $\left\langle k \middle| j\right\rangle = \delta_{kj}$. They form a complete set or a basis.
So any state can be written as a – usually infinite – linear combination of them.
This is also true for the initial state $\left|\Psi(0)\right\rangle$ of the total *perturbed* system:

$$\left|\Psi(0)\right\rangle = \sum_j C_j(0) \left|j\right\rangle .$$

Time dependence of an unperturbed solution

If there is no external action, then the system is closed: $K = 0$.

Then the general solution of $i\hbar\frac{\partial|\Psi(t)\rangle}{\partial t} = H_0\,|\Psi(t)\rangle$ is known from quantum mechanics:

$$|\Psi(t)\rangle = \sum_j c_j(0)e^{-i\frac{\varepsilon_j}{\hbar}t}\,|j\rangle\,.$$

Notes:

1. In the case of degeneracy, the value of ε_j is the same for different orthogonal stationary states $|j\rangle$.
2. If the spectrum H_0 has a continuous part, then $\sum_j$ is to be completed by an integration over the continuous part.
3. Normalization requires $\sum_j |c_j(0)|^2 = 1$.

For a specified initial state $|\Psi(0)\rangle = \sum_j c_j(0)\,|j\rangle$, we have $c_j(0) = \langle j\,|\Psi(0)\rangle$, and the solution corresponding to this initial value is

$$|\Psi(t)\rangle = \sum_j e^{-i\frac{\varepsilon_j}{\hbar}t}\,|j\rangle\,\langle j\,|\Psi(0)\rangle\,.$$

Interaction picture amplitudes

The *perturbation operator* $K(t)$ depends on time. It is also a linear, selfadjoint operator, it will be specified for field-atom interactions later.

It is straightforward to consider the effect of $K(t)$ by looking for the solution of (SchE) in the form:

$$|\Psi(t)\rangle = \sum C_j(t) e^{-i\frac{\varepsilon_j}{\hbar}t} |j\rangle$$

with *time dependent* coefficients $C_j(t)$ instead of the constant values $c_j(0)$.
This time-dependence can be obviously attributed to $K(t)$.

Interaction picture amplitudes

In

$$|\Psi(t)\rangle = \sum C_j(t) e^{-i\frac{\varepsilon_j}{\hbar}t} |j\rangle ,$$

normalization requires:

$$\sum_j |C_j(t)|^2 = 1, \qquad \text{similarly to} \sum_j |c_j(0)|^2 = 1.$$

One says that the expansion coefficients $C_j(t)$ are the amplitudes of $|\Psi(t)\rangle$ in the so-called *interaction picture*.

They are used here instead of the coefficients $c_j(t) = C_j(t)e^{-i\frac{\varepsilon_j}{\hbar}t}$, which are the amplitudes in the *Schrödinger picture*. Soon we come to explain this in more detail.

Interaction picture amplitudes

The equation determining the coefficients $C_j(t)$ follows from the Schrödinger equation $i\hbar\frac{\partial}{\partial t}\left|\Psi(t)\right\rangle = (H_0 + K)\left|\Psi(t)\right\rangle$. We obtain:

$$i\hbar\frac{\partial\left|\Psi(t)\right\rangle_S}{\partial t} = i\hbar\frac{\partial}{\partial t}\sum C_j(t)e^{-i\frac{\varepsilon_j}{\hbar}t}\left|j\right\rangle = \\ = \sum_j (i\hbar\dot{C}_j(t) + \underline{C_j(t)\varepsilon_j})\left|j\right\rangle e^{-i\frac{\varepsilon_j}{\hbar}t} \tag{1}$$

$$(H_0 + K)\left|\Psi(t)\right\rangle_S = \sum_j \underline{C_j(t)e^{-i\frac{\varepsilon_j}{\hbar}t}H_0}\left|j\right\rangle + \sum_j C_j(t)e^{-i\frac{\varepsilon_j}{\hbar}t}K\left|j\right\rangle \tag{2}$$

$$i\hbar\sum_j \dot{C}_j(t)\left|j\right\rangle e^{-i\frac{\varepsilon_j}{\hbar}t} = \sum_j C_j(t)e^{-i\frac{\varepsilon_j}{\hbar}t}K\left|j\right\rangle ,$$

as the underlined terms in (1) and in (2) cancel due to $H_0\left|j\right\rangle = \varepsilon_j\left|j\right\rangle$.

Equation for the interaction picture amplitudes

$$i\hbar \sum_j \dot{C}_j(t) \left|j\right\rangle e^{-i\frac{\varepsilon_j}{\hbar}t} = \sum_j C_j(t) e^{-i\frac{\varepsilon_j}{\hbar}t} K \left|j\right\rangle$$

Multipyling by $e^{i\frac{\varepsilon_k}{\hbar}t} \left\langle k\right|$, and making use of $\left\langle k \middle| j\right\rangle = \delta_{kj}$, we obtain

$$i\hbar \frac{\partial}{\partial t} C_k(t) = \sum_j K_{kj} e^{i\omega_{kj}t} C_j(t) \qquad K_{kj} = \left\langle k\right| K \left|j\right\rangle , \tag{Ck}$$

where $\omega_{kj} = (\varepsilon_k - \varepsilon_j)/\hbar$ are the Bohr frequencies of the unperturbed atom, and K_{kj} are the corresponding matrix elements of the perturbation operator between the unperturbed eigenstates of H_0. This equation determines the $C_k(t)$ interaction picture amplitudes.

Formal introduction of the Interaction picture

In this and in the next two slides in blue, we make a small detour, and give a more formal definition of the interaction picture, also known as Dirac picture.
Blue material is not necessary to understand subsequent slides.

Multiply $|\Psi(t)\rangle$ by the unitary operator $U_0^+ = e^{iH_0 t/\hbar}$ and consider the vectors:

$$|\Psi(t)\rangle_I := e^{iH_0 t/\hbar} |\Psi(t)\rangle \qquad \text{(PsI)}$$

called the state in the interaction picture. In contrast, the usual ket $|\Psi(t)\rangle \equiv |\Psi(t)\rangle_S$ is called the state in the Schrödinger picture, although this is usually not stated explicitly when one begins to learn the Schrödinger equation. We see that

$$|\Psi(t)\rangle_I := e^{iH_0 t/\hbar} |\Psi(t)\rangle_S = e^{iH_0 t/\hbar} \sum C_j(t) e^{-i\frac{\varepsilon_j}{\hbar}t} |j\rangle = \sum C_j(t) |j\rangle .$$

Operators in the Interaction picture

$$|\Psi(t)\rangle_I := e^{iH_0 t/\hbar} |\Psi(t)\rangle_S , \qquad t = 0 : |\Psi(0)\rangle_I = |\Psi(0)\rangle_S .$$

A linear operator denoted until now by A, and from now on by $A_S := A$, is to be called the operator of a physical quantity (observable) in the Schrödinger picture.
With the mapping $A_S |\Psi\rangle_S = |\Psi'\rangle_S$, we prescribe that an analogous equation $A_I |\Psi\rangle_I = |\Psi'\rangle_I$ should hold for the corresponding states in the interaction picture, with an appropriately defined A_I. From (PsI) we get

$$A_S |\Psi\rangle_S = \left|\Psi'\right\rangle_S = A_S e^{-\frac{i}{\hbar}H_0 t} |\Psi\rangle_I = e^{-\frac{i}{\hbar}H_0 t} \left|\Psi'\right\rangle_I .$$

By multiplying the last equality by $e^{\frac{i}{\hbar}H_0 t}$ from the left, we see, that together with $A_S |\Psi\rangle_S = |\Psi'\rangle_S$, the equation $A_I |\Psi\rangle_I = |\Psi'\rangle_I$ also holds, if we *define*

$$A_I := e^{\frac{i}{\hbar}H_0 t} A_S e^{-\frac{i}{\hbar}H_0 t}.$$

Equivalence of the Schrödinger and Interaction pictures

We obtained:

$$A_I := e^{\frac{i}{\hbar}H_0 t} A_S e^{-\frac{i}{\hbar}H_0 t} \quad \Longleftrightarrow \quad A_S = e^{-\frac{i}{\hbar}H_0 t} A_I e^{+\frac{i}{\hbar}H_0 t}.$$

It is simple to show that the expectation values and the commutators of operators are invariant, when we go over to the interaction picture.

Problems:
Show that for any state and operator $\langle \Psi_s | A_S | \Psi_s \rangle = \langle \Psi_I | A_I | \Psi_I \rangle$.
Show that if $[A_S, B_S] = C_S$, *then* $[A_I, B_I] = C_I$ *and the other way around.*

Integral equation for the amplitudes $C_k(t)$

We turn back to (Ck) $i\hbar\frac{\partial}{\partial t}C_k(t) = \sum_j K_{kj}e^{i\omega_{kj}t}C_j(t)$ and recast it into an integral equation.
This has the advantage that the equation contains explicitly the initial conditions, which we fix at $t = 0$:

$$C_k(t) = C_k(0) - \frac{i}{\hbar}\int_0^t \sum_j K_{kj}(t_1)e^{i\omega_{kj}t_1}C_j(t_1)dt_1. \qquad \text{(inteq)}$$

This is only formally a solution for $C_k(t)$, as the unknown amplitudes also figure under the integral sign on the right hand side.
Still it allows us a method of solution, called the *method of successive approximations*, which is especially useful if one has a great number of stationary states.
In the case of a small finite dimensional space, when we have only a few amplitudes, there are other methods to solve for the C_k amplitudes.

Successive approximation

Zeroth approximation: the solutions are taken to be equal to their initial values

$$C_k^{(0)}(t) = C_k(0), \qquad \forall k.$$

This can be valid approximately only for a very short time interval after $t = 0$.
The first approximation is obtained if we replace $C_j(t_1)$ on the right hand side of (inteq) by its zeroth approximation:

$$C_k^{(1)}(t) = C_k(0) - \frac{i}{\hbar}\int_0^t \sum_j K_{kj}(t_1) e^{i\omega_{kj}t_1} C_j^{(0)}(t_1) dt_1 =$$

$$= C_k(0) - \frac{i}{\hbar}\int_0^t \sum_j K_{kj}(t_1) e^{i\omega_{kj}t_1} C_j(0) dt_1.$$

Recursion formula and cut-off

The $(n+1)$th approximation can be expressed by the nth one

$$C_k^{(n+1)}(t) = C_k(0) - \frac{i}{\hbar}\int_0^t \sum_j K_{kj}(t_1) e^{i\omega_{kj}t_1} C_j^{(n)}(t_1) dt_1.$$

In this way we obtain a recursion system for the amplitudes. Explicit expression with sums of multiple integrals can be given, but we omit the complicated expression here.

The nth order amplitude shall depend on the nth power of the perturbing operator K^n. If K is small, i.e. the perturbation is weak, one expects to neglect terms above a certain order. In most of the cases a cutoff is made in the approximation after the first few steps. One expects that this should give good results until the coefficients do not differ too much from their initial values.

Validity of the perturbation series

There are cases when this cutoff cannot be justified at any step, especially in case of resonance, when the amplitudes C change significantly, the perturbation method fails, and other methods are to be used.

For instance, if one of the C-s change from 0 to 1 then we can exploit that all the other C-s must then be close to zero. We postpone this question to Lecture 8.

If we expect that the response of the system is linear to the disturbance, then it is sufficient to make a first-order approximation, as follows now.

A specific initial condition

Assume that initially only one of the amplitudes is nonzero. For instance if the quantum system in question is an atom, then without external perturbation it is in its ground state, and only the ground state amplitude will be different from zero. Let the label of the initial state be $k = i$, so $C_i(0) = 1$.
Then due to the normalization condition $\sum |C_k|^2 = 1$ all the other C_k-s must be 0, i.e. $C_k(0) = \delta_{ik}$.
The integral equation then takes the following simpler form:

$$C_k^{(1)}(t) = \delta_{ik} - \frac{i}{\hbar} \int_0^t K_{ki} e^{i\omega_{ki} t_1} dt_1.$$

First-order perturbation in differential form

Having made the first-order approximation we can also go back now to the differential form of the equation

$$C_k^{(1)}(t) = \delta_{ik} - \frac{i}{\hbar}\int_0^t K_{ki} e^{i\omega_{ki}t_1} dt_1$$

by taking its time derivative, complemented by the initial condition:

$$\frac{dC_k^{(1)}(t)}{dt} = -\frac{i}{\hbar} K_{ki} e^{i\omega_{ki}t}, \qquad C_k^{(1)}(0) = \delta_{ik}.$$

We remind once more that $K_{ki} = \langle k | K_S | i \rangle$ are the matrix elements of the interaction operator (in the Schrödinger picture !) and $\omega_{ki} = (\varepsilon_k - \varepsilon_i)/\hbar$ are the (circular) Bohr frequencies of the possible transitions. In the next lecture we will apply this differential equation to important physical problems.

Questions

1. What are the basic assumptions in time-dependent perturbation theory?
2. What is the time dependence of a single energy eigenstate corresponding to a static Hamiltonian?
3. What are the basic mathematical properties of unitary operators?
4. What is the fundamental difference between Scrödinger, Heisenberg and interaction pictures of quantum mechanics?
5. In the case of time-independent Hamiltonians, what is the form of the unitary operator that connects the Schrödinger and interaction pictures?
6. Show that for any state and operator $\langle \Psi_s | A_S | \Psi_s \rangle = \langle \Psi_I | A_I | \Psi_I \rangle$.

Questions (continued)

7. Show that if $[A_S, B_S] = C_S$, then $[A_I, B_I] = C_I$ and the other way around.
8. Explain the notion of successive approximation in the context of time- dependent perturbation theory.
9. In what cases is it sufficient to perform low-order perturbation calculations?
10. Consider the initial condition of $C_k(0) = \delta_{ik}$. What are the perturbative integral equations in first order?
11. Consider the initial condition of $C_k(0) = \delta_{ik}$. What is the differential form of the first order perturbative equations?
12. Consider the initial condition of $C_k(0) = \delta_{ik}$ and assume that $K_{in} = 0$ for a given state labeled by n. According to first-order perturbation theory, will this state get populated ever? And in higher orders?

Reference

- C. Cohen-Tannoudji, B. Diu, F Laloë, *Quantum Mechanics*, Wiley Interscience (New York, London, Sydney, Toronto) (1977).