

PHYS-E0420 Many-Body Quantum Mechanics

Spring 2024/Päivi Törmä

Outline of the course

What: Time-dependent perturbation theory (Lectures 1-2)

Why: Time-dependent perturbation theory is an integral part of a proper physicist education. It provides the basic quantum mechanical description of a wide range of responses, perturbations and measurements in physics. An example is transitions between electronic states of an atom caused by light, that is, the basics of spectroscopy.

What: Many-body quantum physics (Lectures 3-12)

Why: Many intriguing quantum phenomena that are either already at the application stage or at the forefront of modern research cannot be explained using quantum mechanics for a single system, that is, without taking into account the many-body nature of the system. Examples of phenomena and fields where many-body effects are important are quantized light, quantum optics, superconductivity, other many-body quantum states of matter such as Mott insulators, quantum information, etc.

Methods: In this course, you will learn time-dependent perturbation theory, and the basic many-body quantum methods, such as second quantization. The methods will be systematically used, and used again, throughout the course, so that you will master them by the end of the course.

Physical phenomena: What comes to physical phenomena, the aim is not the same as with methods where we repeat the same things in order to learn them thoroughly. We will not focus on one physical phenomenon or one research field throughout the course, instead, we will give examples and snapshots of various physical phenomena from different research fields. The idea is to give you a broad perspective of the many interesting things that are happening in the present-day studies of quantum many-body phenomena.

Lecture 1

Literature: R.L. Liboff, Introductory Quantum Mechanics (Fourth edition) (Addison Wesley), Chapters 13.5-13.8

Learning goals

- To know the difference between Heisenberg, Schrödinger and Interaction pictures; to be able to make calculations using them.
- To be able to calculate time-development of a quantum system using 1st order perturbation theory; understand the physical meaning of the result for harmonic and adiabatic perturbation.

1 Time-development of quantum systems

From previous courses, you know that the Schrödinger equation describes the time-development of quantum systems. It is, however, in most practical cases impossible to solve exactly. One approach to describe time-development in an approximative way is time-dependent perturbation theory. It is, as the name indicates, similar to

the time-independent perturbation theory that you have already learned in previous courses.

Time-dependence and its perturbative treatment is of special interest when we probe the system. We want to learn about the properties of a quantum system by probing it, i.e. "disturbing" it a bit and seeing how it reacts to it. This kind of disturbance should be weak and not dramatically change the system so that we can treat it as a small perturbation.

When considering time-dependence, it is useful to learn three different ways of formulating the problem of quantum time-evolution: the Schrödinger, the Heisenberg, and the Interaction pictures. These are physically exactly equivalent. You can view them just as the same old Schrödinger equation represented by using different bases. However, from the practical point of view, depending on the system in question, one of them can be the most convenient mathematical formulation of the problem.

Once we have learned these three pictures, we will use the Interaction picture to derive the basic results of time-dependent perturbation theory.

2 Schrödinger, Heisenberg and Interaction pictures

2.1 Schrödinger picture

Note: in these lecture notes, operators are usually not marked with a hat. For instance the Hamiltonian which is marked just H not \hat{H} . However, in some of the lectures some operators are marked with the hat, this is in cases where it might be slightly non-trivial to see what is an operator and what is not.

The Schrödinger picture is what you are the most familiar with from other courses. The Schrödinger equation for the time evolution of the quantum state is

$$i\hbar \frac{d}{dt} |\Psi(t)\rangle = H(t) |\Psi(t)\rangle, \quad (2.1)$$

where $H(t)$ is the Hamiltonian operator that can, indeed, depend on time. For clarity, we add a subindex (S,H,I) to refer to quantum states and operators in a particular picture (Schrödinger, Heisenberg, Interaction):

$$i\hbar \frac{d}{dt} |\Psi(t)\rangle_S = H_S(t) |\Psi(t)\rangle_S. \quad (2.2)$$

Formally one can solve the above equation as

$$|\Psi(t)\rangle_S = U(t) |\Psi(0)\rangle_S, \quad (2.3)$$

where $U(t)$ is the time-evolution operator that propagates the state from time 0 to time t . If the Hamiltonian is time-independent, i.e. $H(t) = H$, the form of $U(t)$ is

$$U(t) = e^{-\frac{i}{\hbar} H t}. \quad (2.4)$$

It is very easy to show (just insert Equations (2.3) and (2.4) into (2.2) and take the time derivative) that this fulfills the Schrödinger equation. If the Hamiltonian is time-dependent, one can write the equation (2.1) in the form

$$|\Psi(t)\rangle_S = |\Psi(0)\rangle_S - \frac{i}{\hbar} \int_0^t dt' H(t') |\Psi(t')\rangle_S. \quad (2.5)$$

Then one can iterate this to obtain the series solution

$$|\Psi(t)\rangle_S = \left[1 - \frac{i}{\hbar} \int_0^t dt' H(t') + \frac{i^2}{\hbar^2} \int_0^t dt' \int_0^{t'} dt'' H(t') H(t'') + \dots \right] |\Psi(0)\rangle_S. \quad (2.6)$$

One can write the time-evolution operator in equation (2.3) in the form

$$U(t) = T e^{-\frac{i}{\hbar} \int_0^t d\tau H(\tau)}, \quad (2.7)$$

where T is the so-called time-ordering operator. The time-ordering operator means that all operators are arranged in such a way that the ones corresponding to earlier times are on the right. As an example for an operator A at different times:

$$T[A(t_1)A(t_2)A(t_3)] = A(t_3)A(t_1)A(t_2) \quad IF \quad t_3 > t_1 > t_2. \quad (2.8)$$

You will derive the result of Equation (2.7) in the **Exercise set 1**. At the moment, you can just think that is a formal way of writing the result of equation (2.6). In general, we can also integrate the Schrödinger equation not from time 0 to time t , but from arbitrary time t_0 to time t . Then the time-evolution operator is denoted by $U(t, t_0)$ and becomes:

$$U(t, t_0) = T e^{-\frac{i}{\hbar} \int_{t_0}^t d\tau H(\tau)} \quad (2.9)$$

and

$$|\Psi(t)\rangle_S = U(t, t_0)|\Psi(t_0)\rangle_S. \quad (2.10)$$

Ultimately we are interested in the observables and their expectation values (i.e. results from the measurements). The expectation value of an observable related to the operator A (A_S in the Schrödinger picture), for instance position, momentum, spin, etc. is

$$\langle A_S(t) \rangle = {}_S \langle \Psi(t) | A_S | \Psi(t) \rangle_S. \quad (2.11)$$

Since we are interested in how this expectation value varies in time, we calculate the equation of motion

$$\begin{aligned} i\hbar \frac{d}{dt} \langle A_S(t) \rangle &= i\hbar \left[\left(\frac{d}{dt} {}_S \langle \Psi(t) | \right) A_S | \Psi(t) \rangle_S + {}_S \langle \Psi(t) | A_S \left(\frac{d}{dt} | \Psi(t) \rangle_S \right) + {}_S \langle \Psi(t) | \left(\frac{dA_S}{dt} \right) | \Psi(t) \rangle_S \right] \\ &= {}_S \langle \Psi(t) | [A_S, H(t)] | \Psi(t) \rangle_S. \end{aligned} \quad (2.12)$$

Here the observable A_S is independent of time $\frac{dA_S}{dt} = 0$. In the Schrödinger picture, operators are always constants in time. But the expectation value does depend on time since the state evolves in time.

However, one can make also another choice: to have the states constant in time, and the operators evolving! This is the Heisenberg picture. This is possible because in quantum mechanics, it is allowed to change the basis by a unitary transformation: such a basis change does not change the physically meaningful quantities, namely observables. Since the time-evolution operator is a unitary operator, we can just apply its inverse, U^{-1} to the time-dependent states of the Schrödinger picture and make them time-independent! However, we have to make the same basis change to operators, and this will make them time-dependent. Let us look closer at this so-called Heisenberg picture.

2.2 Heisenberg picture

In the Heisenberg picture the state remains constant but the operators evolve. We denote the state in the Heisenberg picture by $|\Psi(t)\rangle_H$ and define it from the Schrödinger picture state as

$$|\Psi(t)\rangle_H = U(t)^{-1}|\Psi(t)\rangle_S, \quad (2.13)$$

where we use the basis transformation operator that is the inverse of the time evolution operator, $U(t)^{-1}$. Inserting the time-evolution of $|\Psi(t)\rangle_S = U(t)|\Psi(0)\rangle_S$ into this we see that the state in the Heisenberg representation is indeed independent of time

$$|\Psi(t)\rangle_H = |\Psi(0)\rangle_S =: |\Psi\rangle_H. \quad (2.14)$$

What about the expectation values then? Since we have made a basis transformation, the operators (and observables) also need to be transferred to the new basis

$$A_H(t) = U(t)^{-1}A_S U(t), \quad (2.15)$$

where A_S is the observable A discussed above in the Schrödinger representation. The Hamiltonian operators have this relation as well:

$$H_H(t) = U(t)^{-1}H_S U(t). \quad (2.16)$$

Of course, for time-independent Hamiltonians, $U(t) = e^{-\frac{i}{\hbar}H_S t}$ commutes with H_S and we have simply $H_H = H_S$. However, for time-dependent Hamiltonians, one should use Equation (2.16) in case the Hamiltonians at different times do not commute. It is easy to see that the time-evolution of the expectation value $\langle A(t) \rangle$ is unchanged

$${}_H\langle\Psi|A_H(t)|\Psi\rangle_H = {}_S\langle\Psi(t)|A_S|\Psi(t)\rangle_S. \quad (2.17)$$

Also, the Schrödinger equation of motion for the state will be replaced by a similar looking equation of motion for the operators

$$i\hbar\frac{d}{dt}A_H(t) = i\hbar\frac{d}{dt}(U(t)^{-1}A_S U(t)) = i\hbar\left(\frac{d}{dt}U(t)^{-1}\right)A_S U(t) + U(t)^{-1}A_S i\hbar\left(\frac{d}{dt}U(t)\right). \quad (2.18)$$

In the **Exercise set 1**, you will show that this leads to the so-called *Heisenberg equation of motion*:

$$i\hbar\frac{d}{dt}A_H(t) = -H_H(t)A_H(t) + A_H(t)H_H(t) = [A_H, H_H]. \quad (2.19)$$

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2.3 Interaction picture

Quite often one part of the Hamiltonian H corresponds to a system that we can exactly solve, let us denote it H_0 , and another part, say $V(t)$, to some features that make the system complicated:

$$H = H_0 + V(t). \quad (2.20)$$

For instance, H_0 could describe a particle in a box, a problem to which the solution is exactly known. The other part V could then correspond to, e.g., the interactions of the particle with something else, which in general makes the problem hard to solve. In some cases one can also view that H_0 is the system of interest and V a small perturbation used for probing it. It is often quite practical to solve time-development in such a way that H_0 and V are treated differently. We can make a choice where H_0 gives the time dependence to operators, as in Heisenberg picture, but V then acts like the Hamiltonian in the Schrödinger picture. This approach is called the Interaction picture.

In the Interaction picture, one defines a time-evolution operator U_0 that corresponds to the H_0 part of the Hamiltonian:

$$U_0(t) = T e^{-\frac{i}{\hbar} \int_0^t d\tau H_0(\tau)}. \quad (2.21)$$

The operators are evolved according to this, i.e., according to only part of the Hamiltonian. Quite often $H_0(t)$ is actually time-independent because energy (time-dependence) is given by the perturbation $V(t)$; in the following we will assume so, that is, $H_0(t) = H_0$. In the Heisenberg picture, the quantum state wavefunction became independent of time when such a basis transformation was applied, see Equation (2.14). In the Interaction picture, the wavefunction is not independent of time because U_0 contains only part of the Hamiltonian, i.e. it cannot cancel all the time development of the Schrödinger picture wavefunction:

$$\begin{aligned} |\psi(t)\rangle_I &= e^{iH_0t/\hbar} |\psi(t)\rangle_S \\ &= e^{iH_0t/\hbar} T e^{-\frac{i}{\hbar} \int_0^t d\tau H(\tau)} |\psi(0)\rangle_S \\ &= e^{iH_0t/\hbar} T e^{-\frac{i}{\hbar} \int_0^t d\tau H(\tau)} |\psi(0)\rangle_I. \end{aligned} \quad (2.22)$$

Let us calculate the time derivative of the state

$$\begin{aligned} i\hbar \frac{d}{dt} |\psi(t)\rangle_I &= i\hbar \frac{d}{dt} \left(e^{iH_0t/\hbar} T e^{-\frac{i}{\hbar} \int_0^t d\tau H(\tau)} |\psi(0)\rangle_I \right) \\ &= -H_0 e^{iH_0t/\hbar} T e^{-\frac{i}{\hbar} \int_0^t d\tau H(\tau)} |\psi(0)\rangle_I + e^{iH_0t/\hbar} H(t) T e^{-\frac{i}{\hbar} \int_0^t d\tau H(\tau)} |\psi(0)\rangle_I \\ &= -H_0 |\psi(t)\rangle_I + H_I(t) |\psi(t)\rangle_I \\ &= V_I(t) |\psi(t)\rangle_I, \end{aligned} \quad (2.23)$$

where H_I and V_I are the operators H and V in the interaction picture, obtained through the relation

$$\mathcal{O}_I(t) = e^{iH_0t/\hbar} \mathcal{O} e^{-iH_0t/\hbar}. \quad (2.24)$$

The usefulness of the interaction picture comes apparent when one actually tries to solve the time-evolution of the state. Solving the above differential equation (2.23) yields the time evolution

$$|\Psi(t)\rangle_I = U_I(t) |\Psi(0)\rangle_I, \quad (2.25)$$

where the interaction picture time evolution operator is $U_I(t) = T e^{-\frac{i}{\hbar} \int_0^t d\tau V_I(\tau)}$. To see explicitly the terms of different order in the series expansion, we write $V = \lambda H'$

(see **Exercise set 1**):

$$\begin{aligned}
 U_I(t) = & 1 + \sum_{n=1}^{\infty} \left(\frac{-i\lambda}{\hbar} \right)^n \int_0^t d\tau_n \int_0^{\tau_n} d\tau_{n-1} \dots \int_0^{\tau_2} d\tau_1 \\
 & U_0(0, \tau_n) H'_S(\tau_n) U_0(\tau_n, \tau_{n-1}) H'_S(\tau_{n-1}) \dots U_0(\tau_2, \tau_1) H'_S(\tau_1) U_0(\tau_1, 0).
 \end{aligned}
 \tag{2.26}$$

This forms a convenient basis for the time-dependent perturbation theory:

- H_0 is simple so that $U_0(t)$ is easy to calculate
- all complications go into $V = \lambda H'$
- one can do perturbative theory using the above series expansion, to any order in λ
- First-order (time-dependent) perturbation theory for the wavefunction is obtained by keeping (only) the zero (λ^0) and first (λ^1) order terms in the series expansion of the wavefunction. Note that when calculating any observables in general, one has to take care that all terms in the wavefunction expansion that may lead to an N th order contribution λ^N are included in the expansion; this will be discussed more in the Section 3.2 below.

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In practice the interaction picture may well be the preferred picture since we can seldom handle the time-evolution nonperturbatively. But there are uses for the other pictures too. For some simple systems the time-evolution can be solved exactly, using simply the Schrödinger or Heisenberg equations of motions.

3 Time-dependent perturbation theory

The time-independent perturbation theory (PT) has already been covered in a previous course(s). PT yields the leading order corrections (up to a chosen order) to the eigenstates and the eigenenergies. Time-dependent perturbation theory (TDPT) supplements the time-independent PT by allowing the study of quantum dynamics, or time-evolution, in the presence of a weak perturbation $V(t)$. In particular, it gives the *transition rates* between different eigenstates of the unperturbed Hamiltonian H_0 , for instance, transition rates for transitions between electronic states of an atom when it is perturbed by a light field.

It is important to understand this difference of *time-independent* and *time-dependent* perturbation theories. In the case of a time-independent perturbation $V(t) = V$, PT gives the approximate *eigenstates* of the full Hamiltonian $H_0 + V$ whereas TDPT gives the *time-evolution*.

The basic results of TDPT can be derived in various ways. One can, as is done for instance in Liboff 13.5. and in D.J. Griffiths, Introduction to Quantum Mechanics, calculate the time-evolution of the wavefunction, projecting it to the eigenbasis of H_0 and keeping only terms with low-order in V . An alternative approach is to use the time-evolution of the state in the interaction picture. We use that approach here.

3.1 Interaction picture

The Hamiltonian is written as

$$H = H_0 + V(t), \quad (3.1)$$

where H_0 is simple enough so that we know its eigenstates and $V(t)$ is sufficiently small that treating it using a low-order perturbation theory is justifiable.

The time-evolution of the state (or wavefunction) in the interaction picture $|\psi(t)\rangle_I$ is

$$|\psi(t)\rangle_I = U_I(t, t_0)|\psi(t_0)\rangle_I, \quad (3.2)$$

where we assume that the state at time t_0 is known and is not affected by the perturbation (thus we assume $V(t) = 0$, for $t < t_0$).

The time-evolution operator is given by

$$U_I(t, t_0) = 1 + \frac{1}{i\hbar} \int_{t_0}^t dt' V_I(t') + \left(\frac{1}{i\hbar}\right)^2 \int_{t_0}^t dt' V_I(t') \int_{t_0}^{t'} dt'' V_I(t'') + \dots, \quad (3.3)$$

where $V_I(t') = e^{iH_0(t'-t_0)/\hbar} V(t') e^{-iH_0(t'-t_0)/\hbar}$. This series can be written as

$$U_I(t, t_0) = T e^{-\frac{i}{\hbar} \int_{t_0}^t dt' V_I(t')}. \quad (3.4)$$

The series representation for the time-evolution operator yields the time-dependent perturbation theory. In particular, the first-order time-dependent perturbation theory result for U_I is obtained by approximating

$$U_I(t, t_0) \approx 1 + \frac{1}{i\hbar} \int_{t_0}^t dt' V_I(t'), \quad (3.5)$$

and higher order perturbation theories can be generated in the same way. As with PT, if the second order term does not yield good enough results, it is probably best to try some completely different approach instead of going to third or higher order. But often the first, or at most the second, order theory is sufficient to describe weak perturbations.

3.2 First-order time-dependent perturbation theory

Thus, we obtain the first-order time-dependent perturbation theory result for the wave function

$$|\psi(t)\rangle_I \approx \left[1 + \frac{1}{i\hbar} \int_{t_0}^t dt' V_I(t') + \mathcal{O}((V_I)^2) \right] |\psi(t_0)\rangle_I. \quad (3.6)$$

We are interested in transition probabilities (or probability amplitudes) between different eigenstates of H_0 . These eigenstates yield a nice basis for the interaction picture time-evolution. Assuming that initially the system is in an eigenstate of the unperturbed Hamiltonian H_0 : $|\psi(t_0)\rangle_I = |\psi(t_0)\rangle = |l\rangle$, the probability amplitude for state $|k\rangle$ (also an eigenstate of H_0) at time t is

$$\langle k|\psi(t)\rangle_I \approx \langle k|l\rangle + \frac{1}{i\hbar} \int_{t_0}^t dt' \langle k|V_I(t')|l\rangle + \mathcal{O}((V_I)^2). \quad (3.7)$$

Let us assume that the time-dependence of the perturbation $V(t)$ is factorable, i.e. we can write $V(t) = \lambda H' f(t)$, where H' is an operator but $f(t)$ is simply a

complex valued function. Now we have $V_I(t') = e^{iH_0(t'-t_0)/\hbar} \lambda H' f(t') e^{-iH_0(t'-t_0)/\hbar}$. Assuming also that $k \neq l$, i.e. $\langle k|l \rangle = 0$, we get the probability amplitude

$$\langle k|\psi(t)\rangle_I \approx \frac{\lambda \langle k|H'|l \rangle}{i\hbar} \int_{t_0}^t dt' e^{i(E_k - E_l)(t'-t_0)/\hbar} f(t') + \mathcal{O}((V_I)^2), \quad (3.8)$$

where E_k and E_l are the unperturbed eigenenergies (according to H_0) of the states $|k\rangle$ and $|l\rangle$. The probability for the transition is the absolute value squared of this (we also choose $t_0 = 0$):

$$|\langle k|\psi(t)\rangle_I|^2 \approx \frac{\lambda^2 |\langle k|H'|l \rangle|^2}{\hbar^2} \left| \int_0^t dt' e^{i(E_k - E_l)t'/\hbar} f(t') \right|^2 + \mathcal{O}((V_I)^3). \quad (3.9)$$

This equation is the same as Eq.13.52 in Liboff (with $t_0 = -\infty$). Note that the assumption $\langle k|l \rangle = 0$ was essential: if that is not valid, one should include explicitly the term of the order V_I^2 in the wavefunction expansion (3.6) because it would contribute to the result (3.9) when multiplied with the zeroth order term $\langle k|l \rangle$. This is an example of what was already stated above: when calculating any observables in general, one has to take care that all terms in the wavefunction expansion that may lead to an N th order contribution λ^N are included in the expansion. Next we will consider a few important examples.

3.3 Harmonic perturbation

Harmonic perturbation is a very typical one in many contexts, a famous example is light or other electromagnetic radiation (harmonic dependence on frequency, $\cos(\omega t)$) interacting with matter. Assume that the time-dependence of the perturbation is of the form $f(t) = 2 \cos \omega t$, for $t \geq 0$ and $f(t) = 0$, for $t < 0$. (That is, we can define $t_0 = 0$.) Now we get the transition probability amplitude

$$\langle k|\psi(t)\rangle_I \approx \frac{\lambda \langle k|H'|l \rangle}{i\hbar} \int_0^t dt' e^{i(E_k - E_l)t'/\hbar} \left(e^{i\omega t'} + e^{-i\omega t'} \right), \quad (3.10)$$

which yields

$$\langle k|\psi(t)\rangle_I \approx -i2\lambda H'_{kl} \left[\frac{e^{i(E_k - E_l - \hbar\omega)t/(2\hbar)} \sin\left(\frac{E_k - E_l - \hbar\omega}{2\hbar} t\right)}{E_k - E_l - \hbar\omega} + \frac{e^{i(E_k - E_l + \hbar\omega)t/(2\hbar)} \sin\left(\frac{E_k - E_l + \hbar\omega}{2\hbar} t\right)}{E_k - E_l + \hbar\omega} \right]. \quad (3.11)$$

The harmonic perturbation $\lambda H' \cos \omega t$ is a semi-classical approximation of the photon absorption/emission process for a single atom. The first term in the transition probability describes absorption of the photon of energy $\hbar\omega$ and the latter term describes emission of the photon. We could also calculate the transition probability amplitude $k \rightarrow l$ by simply swapping k and l states. This gives the full semiclassical picture of a two-level atom in the presence of the photon field (we are still missing spontaneous emission which is an effect that comes about when we quantize also the light field, as will be done later in this course), with transitions $k \rightarrow l + \text{photon}$ emission/absorption and $l \rightarrow k + \text{photon}$ emission/absorption. Out of these four processes usually only two are (nearly) resonant (in the sense of energy conservation) and two are clearly non-resonant. To understand the relation to time-energy uncertainty, see **Exercise set 1**.

3.4 Adiabatic perturbation

Integrating the Eq. (3.8) by parts one obtains (and assuming $f(t_0) = 0$)

$$\langle k|\psi(t)\rangle_{\text{I}} \approx -\frac{\lambda\langle k|H'|l\rangle}{E_k - E_l} \left[f(t)e^{i(E_k - E_l)(t - t_0)/\hbar} - \int_{t_0}^t dt' e^{i(E_k - E_l)t'/\hbar} \frac{\partial}{\partial t'} f(t') \right]. \quad (3.12)$$

If the perturbation is slowly varying, the first term on the right dominates and we obtain

$$\langle k|\psi(t)\rangle_{\text{I}} \approx -\frac{\lambda\langle k|H'|l\rangle f(t)}{E_k - E_l} e^{i(E_k - E_l)(t - t_0)/\hbar}. \quad (3.13)$$

This is precisely (assuming $f(t)$ almost constant for a particular time interval) the result obtained from time-independent perturbation theory, except for the time-dependent phase factor. The region of validity of the adiabatic approximation will be discussed in **Exercise set 2**.