Exercises III

November 4th

A3.1 *Two state problem*

There are only very few cases in which a problem with a time-dependent potential can be solved exactly and where one does not need to use perturbation theory.. Consider a system with Hamiltonan H_0 and two states $|1\rangle$ and $|2\rangle$ with energies $E_1 < E_2$.

(1) Show that

$$H_0 = E_1|1\rangle\langle 1| + E_2|2\rangle\langle 2|.$$

(2) Since $V(t)$ and thus $H = H_0 + V(t)$ are time-dependent, the problem is no longer stationary, in particular the time evolution operator is not $\mathrm{e}^{-\mathrm{i}Ht/\hbar}$ anymore. Therefore, one switches to the so-called *interaction picture*. Show that for a state

$$|\alpha(t)\rangle_I := \mathrm{e}^{\mathrm{i}H_0 t/\hbar}|\alpha(t)\rangle$$

one has:

$$\mathrm{i}\hbar\frac{\partial}{\partial t}|\alpha(t)\rangle_I = V_I(t)|\alpha(t)\rangle_I \quad \text{with} \quad V_I(t) = \mathrm{e}^{\mathrm{i}H_0 t/\hbar}V(t)\,\mathrm{e}^{-\mathrm{i}H_0 t/\hbar}.$$

In particular, $|\alpha(t)\rangle_I$ remains unchanged for $V = 0$.

(3) In addition, show that $\frac{\mathrm{d}}{\mathrm{d}t}V_I(t) = \frac{1}{\mathrm{i}\hbar}[V_I(t), H_0] + \frac{\partial}{\partial t}V_I(t)$.

(4) The interaction picture, where the timedependence is distributed to both states and operators, may be mixed up with the *Heisenberg picture*, there one defines (for constant H) the operators as $A_H(t) = \mathrm{e}^{\mathrm{i}Ht/\hbar}A\,\mathrm{e}^{-\mathrm{i}Ht/\hbar}$, i.e. with the full H, whereas the states stay unchanged in time. Show the so-called Heisenberg equation of motion $\frac{\mathrm{d}}{\mathrm{d}t}A_H(t) = \frac{1}{\mathrm{i}\hbar}[A_H(t), H] + \frac{\partial}{\partial t}A_H(t)$, again the full H appears.

(5) Now, write $|\alpha(t)\rangle_I$ in terms of the basis $|n\rangle$:

$$|\alpha(t)\rangle_I = \sum_n c_n(t)|n\rangle.$$

Deduce the coupled differential equation system

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}c_n(t) = \sum_m \langle n|V(t)|m\rangle \mathrm{e}^{\mathrm{i}\frac{E_n - E_m}{\hbar}t}c_m(t) =: \sum_m V_{nm}(t)\mathrm{e}^{\mathrm{i}\omega_{nm}t}c_m(t).$$

(6) Let $V(t) = \gamma\,\mathrm{e}^{\mathrm{i}\omega t}|1\rangle\langle 2| + \gamma\,\mathrm{e}^{-\mathrm{i}\omega t}|2\rangle\langle 1|$, where $\gamma, \omega > 0$, be a sine-like potential. What does the presence of this potential cause?

(7) At $t = 0$ let the system be in the state $|1\rangle$: $c_1(0) = 1$, $c_2(0) = 0$. Solve the equation system from (5) for the potential from (6) and obtain *Rabi's formula*

$$|c_2(t)|^2 = \frac{\frac{\gamma^2}{\hbar^2}}{\frac{\gamma^2}{\hbar^2} + \frac{(\omega-\omega_{21})^2}{4}}\sin^2\left(\sqrt{\frac{\gamma^2}{\hbar^2} + \frac{(\omega - \omega_{21})^2}{4}}\;t\right), \quad |c_1(t)|^2 = 1 - |c_2(t)|^2.$$

(8) Interpret the result. When is the oscillation particularly large?

(9) An example for such a system is spin resonance, a particle with spin $\frac{1}{2}$ in a magnetic field $\vec{B} = B_0\vec{e}_3 + B_1(\vec{e}_1\cos\omega t + \vec{e}_2\sin\omega t)$, i.e. a constant, homogeneous field in z direction, superposed by a field rotation in the xy plane. State H_0 and $V(t)$. Which quantity does play the role of γ?

In experiment, such a rotating field is difficult to produce, one takes a field oscillating in x direction instead. This can be written as superposition of a clockwise and a counterclockwise rotating field, where the change of rotational direction is given by $\omega \to -\omega$. Due to the resonance condition $\omega \approx \omega_{21}$, only one of the two components is really relevant.

Homework III

Return: November 11th

H3.1 *Excitation of an atom by collision with a heavy charged particle*

The motion $\vec{R}(t)$ of a heavy particle (charge Z) is quasiclassical, thus the particle moves on a straight line, uniformly with the constant velocity v, e.g. $\vec{R}(t) = (vt, b, 0)$. The potential of the interaction between an electron of an hydrogen atom (with nucleus at the origin) and the particle reads: $\widetilde{V}(t) = -\frac{Ze^2}{|\vec{R}(t)-\vec{r}\,|}$.

(1) Show that a potential not depending on $\vec{r}$ only influences the phase of the wave function of the electron. Thus we do our computation with $V(t) = \widetilde{V}(t) + \frac{Ze^2}{|\vec{R}(t)|}$.

(2) Show that for $|\vec{R}(t)| \gg |\vec{r}\,|$, taking into account dipole and quadrupole, we have

$$V(t) \approx -Ze^2 \left(\frac{vtx_1 + bx_2}{|\vec{R}(t)|^3} + \frac{2x_1^2 - x_2^2 - x_3^2}{2|\vec{R}(t)|^3} + \frac{3b^2(x_2^2 - x_1^2)}{2|\vec{R}(t)|^5} + \frac{3vtbx_1x_2}{|\vec{R}(t)|^5} \right).$$

(3) The transition probability $w_{nm}^{(1)}$ from the state $|m\rangle$ to the state $|n\rangle$ reads

$$w_{nm}^{(1)} = |c_{nm}^{(1)}|^2, \quad c_{nm}^{(1)} = -\frac{\mathrm{i}}{\hbar} \int_{-\infty}^{\infty} \mathrm{d}t \langle n|V(t)|m\rangle\, \mathrm{e}^{\frac{\mathrm{i}(E_m - E_n)t}{\hbar}}$$

in first order time dependent perturbation theory. Show with $\omega = \frac{E_m - E_n}{\hbar}$ that

$$c_{nm}^{(1)} = \frac{\mathrm{i}}{\hbar} Ze^2 \int \Bigg(\frac{|\omega|}{v^2} \left(2x_2 + \frac{2x_1^2 - x_2^2 - x_3^2}{b} \right) K_1\left(\frac{b|\omega|}{v}\right) + \frac{\omega^2}{v^3}(x_2^2 - x_1^2) K_2\left(\frac{b|\omega|}{v}\right)$$
$$+ 2\mathrm{i} \left(\frac{\omega}{v^2} x_1 K_0\left(\frac{b|\omega|}{v}\right) + \mathrm{sign}(\omega) \frac{\omega^2}{v^3} x_1 x_2 K_1\left(\frac{b|\omega|}{v}\right) \right) \Bigg) \psi_n^*(\vec{r}) \psi_m(\vec{r}) \mathrm{d}^3 r,$$

$$\text{where} \quad K_n(\alpha z) = \frac{\Gamma(n + \frac{1}{2})(2z)^n}{\sqrt{\pi}\, \alpha^n} \int_0^{\infty} \frac{\mathrm{d}t \cos(\alpha t)}{(t^2 + z^2)^{n+\frac{1}{2}}}, \quad \alpha > 0.$$

(4) Discuss the value of the transition amplitude $c_{mn}^{(1)}$ for the inverse process.

(5) Estimate the size of the argument $\frac{b|\omega|}{v}$ of the modified Bessel functions K_i. Compare the orders of magnitude of the contributions of dipole and quadrupole to $c_{nm}^{(1)}$. Estimate the coordinates by Bohr's radius and use the asymptotic behaviour $K_n(z) \sim \frac{\mathrm{e}^{-z}}{\sqrt{z}}$ $(z \to \infty)$ and $K_n(z) \sim z^{-n}$, $K_0(z) = -\ln z$ $(z \to 0)$.

(6) With the help of the Wigner/Eckart theorem decide between which states the dipole and quadrupole term in $V(t)$ makes transitions possible (cf. H2.2.4).

(7) Compute with (3) and (6) $c_{2\ell m,1s}^{(1)}$ explicitly and discuss the result.

(30 points)