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 Hamiltonian $H_0$ 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 $e^{-iHt/\hbar}$ anymore. Therefore, one switches to the so-called interaction picture. Show that for a state

$$|\alpha(t)\rangle_I := e^{iH_0t/\hbar}|\alpha(t)\rangle$$

one has:

$$i\hbar \frac{\partial}{\partial t} |\alpha(t)\rangle_I = V_I(t)|\alpha(t)\rangle_I \quad \text{with} \quad V_I(t) = e^{iH_0t/\hbar}V(t)e^{-iH_0t/\hbar}.$$

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

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

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

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

6. Let $V(t) = \gamma e^{i\omega t}|1\rangle\langle 2| + \gamma e^{-i\omega t}|2\rangle\langle 1|$, 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

$$|c_2(t)|^2 = \frac{\gamma^2}{\hbar^2 + (\omega - \omega_2)^2} \sin^2 \left(\frac{\sqrt{\gamma^2 + (\omega - \omega_2)^2}}{4} t\right), \quad |c_1(t)|^2 = 1 - |c_2(t)|^2.$$

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 $\vec{B} = B_0\hat{z}_3 + B_1(\vec{e}_3 \cos \omega t + \vec{e}_5 \sin \omega t)$, 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 $\gamma$?
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 \(\omega \rightarrow -\omega\). Due to the resonance condition \(\omega \approx \omega_2\), only one of the two components is really relevant.

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**Homework III**  
Return: November 11th

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

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

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

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

\[
V(t) \approx -Ze^2 \left( \frac{vt x_1 + bx_2}{|\mathbf{R}(t)|^3} + \frac{2x_1^2 - x_2^2 - x_3^2}{2|\mathbf{R}(t)|^5} + \frac{3x_2^2(x_3^2 - x_1^2)}{2|\mathbf{R}(t)|^5} + \frac{3vtbx_1x_2}{|\mathbf{R}(t)|^5} \right).
\]

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

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

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

\[
c_{nm}^{(1)} = \frac{i}{\hbar} Ze^2 \int \left( \frac{|\omega|}{v^2} \left( 2x_2 + \frac{2x_1^2 - x_2^2 - x_3^2}{b} \right) K_1 \left( \frac{|\omega|}{v} \right) + \frac{\omega^2}{v^3} (x_2^2 - x_1^2) K_2 \left( \frac{|\omega|}{v} \right) \right)
\]

\[
+ 2i \left( \frac{\omega}{v^3} x_1 K_0 \left( \frac{|\omega|}{v} \right) + \text{sign}(\omega) \frac{\omega^2}{v^3} x_1 x_2 K_1 \left( \frac{|\omega|}{v} \right) \right) \psi_n^{*}(r) \psi_m(r) d^3r,
\]

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

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

5. Estimate the size of the argument \(\frac{|\omega|}{v}\) 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 \(K_n(z) \sim \frac{e^{-z}}{\sqrt{\pi}z^n}(z \to \infty)\) 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)