Technische Universität München **Theoretische Physik T70**
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Quantum Mechanics II

Winter Term 2015/16

Hand in until Thursday, 26.11.15, 12:00 next to PH 3218.

Exercise Sheet No. 06 To be discussed from 30.11. - 04.12.15.

Problem 1: Landau-Zener Formula **10 Points**

Consider a two-level quantum mechanical system described by the following time-dependent Hamiltonian

$$H(t) = \begin{pmatrix} -\epsilon(t) & -f \\ -f & \epsilon(t) \end{pmatrix} , \tag{1}$$

with a linearly time-dependent sweep $\epsilon(t) = -\alpha t$ for $\alpha > 0$ and where $f > 0$ is a coupling between the two eigenstates $|1\rangle$ and $|2\rangle$ of the unperturbed system.

(a) Calculate the eigenvalues $E_{1,2}$ of this Hamiltonian and express them in terms of $\epsilon(t)$. Give the eigenvectors $|1\rangle$, $|2\rangle$ and the eigenvalues $E_{1,2}^{\infty}$ at large times $t \to \pm\infty$. Sketch $E_{1,2}(t)$ in the range $-\infty < t < \infty$. What happens for $f \to 0$?

(b) Consider a general state

$$|\psi(t)\rangle = c_1(t)|1\rangle + c_2(t)|2\rangle \tag{2}$$

and show that solving the Schrödinger equation (assume $\hbar \equiv 1$) leads to the ordinary differential equation

$$\frac{d^2}{dt^2} c_2(t) + \left[f^2 - \mathrm{i}\alpha + (\alpha t)^2\right] = 0 \,, \tag{3}$$

for the amplitude $c_2(t)$.

(c) Show that the variable substitution $t \to z(t) = \mathrm{e}^{-\mathrm{i}\frac{\pi}{4}}\sqrt{2\alpha} t$ transforms Eq. (3) to the so-called *Weber equation*,

$$\frac{d^2}{dz^2} \tilde{c}_2(z) + \left[\nu + \frac{1}{2} - \frac{z^2}{4}\right] = 0 \,, \tag{4}$$

with $\nu = \frac{\mathrm{i}f^2}{2\alpha}$ and where $\tilde{c}_2(z) = c_2(z(t))$.

(d) Eq. (4) is solved by the four parabolic cylinder functions, or *Weber functions*, $D_\nu(z)$, $D_\nu(-z)$, $D_{-\nu-1}(iz)$ and $D_{-\nu-1}(-iz)$ the former two of which are linearly independent for $\nu \notin \mathbb{Z}$.
Verify that $D_\mu(\zeta)$ is a solution of the *Weber equation* (4) with $\nu = \mu$ if it obeys the following recursive relations for arbitrary ζ and μ:

$$D_{\mu+1}(\zeta) - \zeta D_\mu(\zeta) + \mu D_{\mu-1}(\zeta) = 0 \,, \tag{5}$$

$$\frac{d}{d\zeta} D_\mu(\zeta) + \frac{1}{2}\zeta D_\mu(\zeta) - \mu D_{\mu-1}(\zeta) = 0 \,. \tag{6}$$

Assume that initially the system is in the state $|1\rangle$, so that the following initial conditions hold:

$$|c_1(t \to -\infty)|^2 = 1\,, \tag{7}$$
$$|c_2(t \to -\infty)|^2 = 0\,. \tag{8}$$

During the linear sweep over the avoided crossings, the coupling f causes population transfer from $|1\rangle$ to $|2\rangle$. Our aim is to find the probability to find system in the state $|1\rangle$ at $t \to \infty$:

$$P_{\mathrm{LZ}} \equiv |c_1(t \to \infty)|^2 = 1 - |c_2(t \to \infty)|^2\,. \tag{9}$$

Among the four solutions of Eq. (4) only the *Weber function* $D_{-\nu-1}(-iz)$ vanishes for $t \to -\infty$. The coefficient $c_2(t)$ thereby fulfills the initial condition (8) if it is written as

$$c_2(t) = \tilde{c}_2(z) = AD_{-\nu-1}(-iz(t))\,, \tag{10}$$

where A is a normalization constant. Defining $R = \sqrt{2\alpha}t$, the asymptotic expressions for $D_{-\nu-1}(-iz(t))$ in the limits $t \to \mp\infty$ are given by

$$D_{-\nu-1}(-iz(t \to -\infty)) = \mathrm{e}^{-\frac{1}{4}\pi(\nu+1)\mathrm{i}}\mathrm{e}^{-\mathrm{i}\frac{R^2}{4}}R^{-\nu-1}\,, \tag{11}$$
$$D_{-\nu-1}(-iz(t \to +\infty)) = \frac{\sqrt{2\pi}}{\Gamma(\nu+1)}\mathrm{e}^{\frac{1}{4}\pi\nu\mathrm{i}}\mathrm{e}^{\mathrm{i}\frac{R^2}{4}}R^{\nu}\,. \tag{12}$$

(e) Find the asymptotic expression $c_1(t \to -\infty)$ by inserting $c_2(t \to -\infty)$ into the Schrödigner equation.

(f) Show that $A = \sqrt{\gamma}\mathrm{e}^{-\frac{\pi\gamma}{4}}$ fulfills the normalization condition (7), where $\gamma = -\mathrm{i}\nu = \frac{f^2}{2\alpha}$.

(g) Derive the *Landau-Zener formula*:

$$P_{\mathrm{LZ}} = \mathrm{e}^{-2\pi\gamma}\,, \tag{13}$$

by using the properties of the *Gamma function*:

$$\Gamma(\pm\mathrm{i}\gamma + 1) = \pm\mathrm{i}\gamma\Gamma(\pm\mathrm{i}\gamma)\,, \tag{14}$$
$$|\Gamma(\pm\mathrm{i}\gamma)| = \sqrt{\frac{\pi}{\gamma\sinh\pi\gamma}}\,. \tag{15}$$

(h) What is the physical consequence for a strong coupling f and a slow variation of the energy difference α, *i.e.* $f^2 \gg \alpha$? What happens for a vanishing coupling f?