FYS 4110 Modern Quantum Mechanics, Fall Semester 2016

Problem set 4

4.1 Spin operators and Pauli matrices

A spin half operator $\hat{\mathbf{S}}$ is defined in the standard way as

$$\hat{\mathbf{S}} = \frac{\hbar}{2}\boldsymbol{\sigma} \tag{1}$$

where $\boldsymbol{\sigma}$ is a vector with the three Pauli matrices $(\sigma_1, \sigma_2, \sigma_3)$ (or equivalently written as $(\sigma_x, \sigma_y, \sigma_z)$) as Cartesian components. We use the standard expressions for these 2x2 matrices, as given in the lecture notes. We also introduce the rotated Pauli matrix, defined by $\sigma_{\mathbf{n}} = \mathbf{n} \cdot \boldsymbol{\sigma}$, where $\mathbf{n}$ is an unspecified three dimensional unit vector.

a) Show that $\sigma_{\mathbf{n}}$ has eigenvalues ± 1, and the eigenstate (in matrix form) corresponding to the eigenvalue $+1$ is (up to an arbitrary phase factor)

$$\Psi_{\mathbf{n}} = \begin{pmatrix} \cos\frac{\theta}{2} \\ e^{i\phi}\sin\frac{\theta}{2} \end{pmatrix} \tag{2}$$

with (θ, ϕ) as the polar angles of the unit vector $\mathbf{n}$. Also show the relation

$$\Psi^{\dagger}_{\mathbf{n}}\boldsymbol{\sigma}\Psi_{\mathbf{n}} = \mathbf{n} \tag{3}$$

b) Show, by using operator identities from Problem Set 2, the following relation

$$e^{-\frac{i}{2}\alpha\sigma_z}\,\sigma_x\,e^{\frac{i}{2}\alpha\sigma_z} = \cos\alpha\,\sigma_x + \sin\alpha\,\sigma_y \tag{4}$$

Explain why this shows that the unitary matrix

$$\hat{U} = e^{-\frac{i}{2}\alpha\sigma_{\mathbf{n}}} = e^{-\frac{i}{\hbar}\alpha\mathbf{n}\cdot\hat{\mathbf{S}}} \tag{5}$$

induces a spin rotation of angle α about the axis $\mathbf{n}$.

c) Demonstrate, by expansion of the exponential function, the following identity

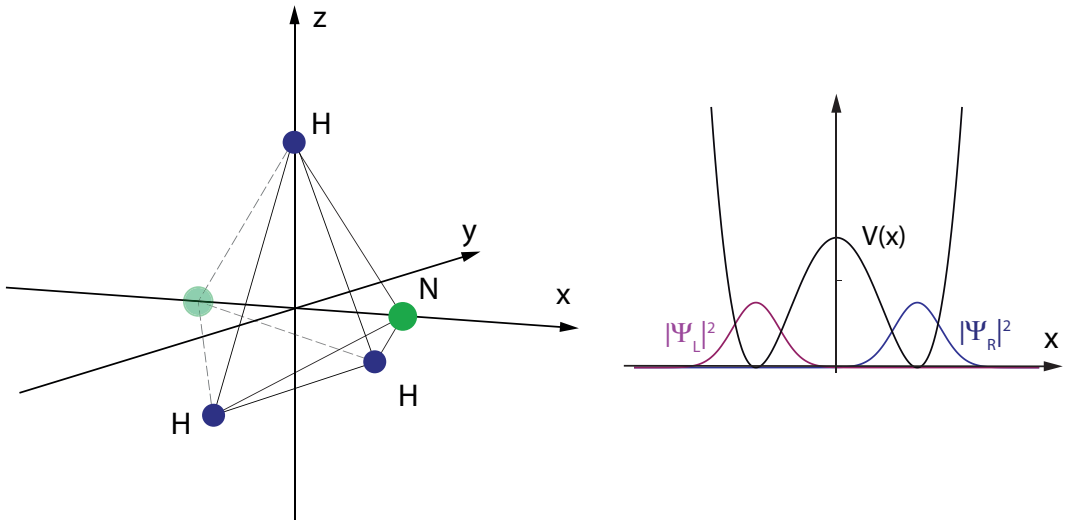
$$e^{-\frac{i}{2}\alpha\sigma_{\mathbf{n}}} = \cos\frac{\alpha}{2}\mathbb{1} - i\sin\frac{\alpha}{2}\sigma_{\mathbf{n}} \tag{6}$$

with $\mathbb{1}$ as the 2x2 identity matrix.

4.2 Oscillations in ammonia molecules (Midterm Exam 2010)

The ammonia molecule has the chemical formula NH_3, which means that it is composed of three hydrogen and one nitrogen atoms. The left part of the figure shows the spatial structure of the molecule, where the hydrogen atoms define a planar, equilateral triangle (in the yz-plane) and the nitrogen atom is located on the orthogonal symmetry axis (x-axis) at some distance from the plane of the hydrogen atoms.

With the plane of the hydrogen atoms being fixed, there are, however, two possible positions of the nitrogen atom that are equally favored with respect to potential energy. They are located symmetrically about the plane, as indicated in the figure.



In the quantum description we associate two different state vectors $|\psi_R\rangle$ and $|\psi_L\rangle$ with these two positions of the nitrogen atom. In the right part of the figure the situation is pictured with the potential energy and the two wave functions shown as functions of the position of the nitrogen atom along the symmetry axis. The potential has the form of a double well with two degenerate ground state positions. With $\hat{H}$ as the Hamiltonian we write this degeneracy as

$$\langle\psi_L|\hat{H}|\psi_L\rangle = \langle\psi_R|\hat{H}|\psi_R\rangle \equiv E_0 \tag{7}$$

There is however a correction to this picture. Even though there is potential barrier between the two equilibrium positions, there is a small probability for quantum tunneling from one position to the other. This is represented by a non-vanishing matrix element

$$\langle\psi_L|\hat{H}|\psi_R\rangle \equiv \lambda \tag{8}$$

were we may assume λ to be real and positive. The value of this matrix element is very small, which means that the corresponding transition time from one minimum of the potential to the other is very long, but the result is that if the nitrogen atom initially is in one of the wells it will oscillate back and forth between the two minima at a low frequency (compared to other atomic frequencies).

The true ground state is however a stationary state, which to a good approximation is a superposition of the states $|\psi_L\rangle$ and $|\psi_R\rangle$ associated with the two minima. In the following we restrict the description to the two-dimensional Hilbert space spanned by these two vectors.

a) Write the Hamiltonian as a 2×2 matrix and find the energy eigenvalues $E_0^{\pm}$ and eigenstates $|\psi_0^{\pm}\rangle$, when the λ terms are included. Express the ground state $|\psi_0^{-}\rangle$ and the excited state $|\psi_0^{+}\rangle$ as linear combinations of $|\psi_L\rangle$ and $|\psi_R\rangle$ and describe briefly with words the characteristics of the two energy eigenstates.

The ammonia molecule has an electric dipole moment which arises from the tendency of the nitrogen atom to attract an electron from the hydrogen atoms. The dipole moment is directed along the symmetry axis in the opposite direction of the nitrogen atom. We assume now that the ammonia molecule is located in a constant electric field $\mathcal{E}$ directed along the x-axis. The field introduces a new term $\hat{H}_d$ in the Hamiltonian with matrix elements

$$\langle\psi_L|\hat{H}_d|\psi_L\rangle \quad = \quad -\langle\psi_R|\hat{H}_d|\psi_R\rangle \equiv \Delta$$

$$\langle\psi_L|\hat{H}_d|\psi_R\rangle \quad = \quad \langle\psi_R|\hat{H}_d|\psi_L\rangle = 0 \tag{9}$$

with $\Delta = \mathcal{E}\, d$, and with d as the electric dipole moment of the molecule.

b) Determine the new energy eigenvalues $E_\pm$ with this additional term in the Hamiltonian, and make a plot that shows how the two energy levels change with variable Δ from a large negative to a large positive value (from $\Delta << -\lambda$ to $\Delta >> \lambda$). Choose $E_\pm/\lambda$ and Δ/λ as variables.

c) Determine eigenvectors $|\psi_\pm\rangle$ expressed in terms of $|\psi_L\rangle$ and $|\psi_R\rangle$ and plot, as functions of Δ, the overlaps $|\langle\psi_L|\psi_\pm\rangle|^2$ between the energy eigenvectors and $|\psi_L\rangle$.

The situation we have here is sometimes referred to as an *avoided crossing* between the two energy levels. Give a brief qualitative description of the crossing based on the plotted curves.

We next assume the electric field to vary periodically with time, $\mathcal{E} = \mathcal{E}_0 \cos\omega t$, and correspondingly, $\Delta = \Delta_0 \cos\omega t$, with Δ_0 as a positive constant.

d) Show that in the $\{|\psi_0^\pm\rangle\}$ basis the Hamilton can be expressed as

$$\hat{H} = E_0 \mathbb{1} + \lambda\sigma_z + \Delta_0 \cos\omega t \sigma_x \tag{10}$$

with σ_x and σ_z as standard Pauli matrices.

The last term in (10) can be written as

$$\Delta_0 \cos\omega t \sigma_x = \frac{1}{2}\Delta_0(e^{i\omega t}\sigma_- + e^{-i\omega t}\sigma_+) + \frac{1}{2}\Delta_0(e^{-i\omega t}\sigma_- + e^{+i\omega t}\sigma_+) \tag{11}$$

where $\sigma_\pm = \frac{1}{2}(\sigma_x \pm i\sigma_y)$ can be viewed as raising and lowering operators in the spectrum of the two-level Hamiltonian. Assuming ω to be positive the first term will usually give the most important contribution to the Hamiltonian. This motivates the so-called *rotating wave approximation*, where the last term in (11) is ommitted. In the following apply this approximation with the Hamiltonian given by

$$\hat{H} = E_0 \mathbb{1} + \lambda\sigma_z + \frac{1}{2}\Delta_0(e^{i\omega t}\sigma_- + e^{-i\omega t}\sigma_+) \tag{12}$$

e) Show that this has the same form as the spin Hamiltonian in a rotating magnetic field, discussed in Sect.1.3.2 of the lecture notes. Outline the method used to find the time evolution operator and give the expressions for the Rabi frequency Ω and resonance frequency ω_0 in terms of the parameters λ and Δ_0. It may be convenient here to re-define the zero-point of the energy so that $E_0 = 0$. Comment on why the value of E_0 is not important. It is sufficient to refer to results from the lecture notes without a detailed derivation.

f) Initially, at time $t = 0$, the system is in the left shifted state $|\psi_L\rangle$. Determine the time dependence of the overlap of the time evolved state $|\psi(t)\rangle$ with the right shifted state, $\langle\psi_R|\psi(t)\rangle$.

g) Assuming that the strength of the oscillating field is given by $\Delta_0 = 2\lambda$, examine numerically the time dependent function $|\langle\psi_R|\psi(t)\rangle|^2$ by making a plot over several periods of this function, for two different values of the frequency, 1) at resonance, $\omega = \omega_0$ and 2) off resonance with $\omega = \omega_0/10$. Use the dimensional variable $\tau = 2\pi\lambda t$ as time coordinate. Make a (qualitative) discussion of what the curves show and compare with the related curve in the case when the electric field is turned off, $\Delta_0 = 0$.