6. gyakorlat (okt. 22)

1. Consider the Hamiltonian of a spin 1/2 particle in a magnetic field parallel to the z axis:

$$H = H_0\mathbb{I} - \frac{qB_z}{m}S_z \tag{1}$$

The systems stays in its ground state until a homogenous magnetic field is turned on along the x direction, $W(t) = -\frac{qB_x}{m}S_x\cos(\omega t)$

(a) Express the perturbation in interaction picture!

Time-evolution of operators are generated by the initial Hamiltonian, that is:

$$U(t,0) = e^{-\frac{i}{\hbar}Ht} = e^{-\frac{i}{\hbar}H_0}e^{\frac{i}{\hbar}\frac{qB_z}{m}S_z} \tag{2}$$

From here we can calculate the effect of the time-evolution on $W(t)$, using the commutation relation, $[S_z, S_x] = i\hbar S_y$ and $[S_z, S_y] = -i\hbar S_x$. Further more also exploiting that spin-diagonal part $e^{-\frac{i}{\hbar}H_0\mathbb{I}t}$ commutes with S_x we get by applying the Haussdorf expansion, $e^ABe^{-A} = B + [A,B] + \frac{1}{2!}[A,[A,B]] + \ldots$: Now take the Schrödinger-equation in interaction picture:

$$i\hbar\partial_t|\psi^D(t)\rangle = W^D(t)|\psi^D(t)\rangle \tag{3}$$

Introducing the time-evolution operator, $U^D(t,0)|\psi(0)\rangle = |\psi^D(t)\rangle$ we have the following equation for it:

$$i\hbar\partial_t U^D(t,0) = W^D(t)U^D(t,0) \tag{4}$$

$$\Rightarrow U^{D(1)}(t,0) = \mathbb{I} - \frac{i}{\hbar}\int_0^t \mathrm{d}t' W^D(t') \tag{5}$$

Starting from one of the system's eigenstates, $|\varphi_i\rangle \otimes \chi_\alpha$ we have for the occupation amplitudes:

$$c_n^{(1)}(t) = \delta_{ni} - \frac{i}{\hbar}\int_0^t \mathrm{d}t' \langle\varphi_n|W^D(t')|\varphi_i\rangle \tag{6}$$

The eigenstates of the inital Hamiltonians are the eigenstates of the H_0 Hamiltonians in the tensor product with the spinor Hilber space, that is $|\varphi_{n,+}\rangle = |n\rangle \otimes \chi_+$ and $|\varphi_{n,-}\rangle = |n\rangle \otimes \chi_-$ with $\chi_- = \begin{pmatrix}0\\1\end{pmatrix}$ and $\chi_+ = \begin{pmatrix}1\\0\end{pmatrix}$ spin up and down states. Now exploiting the fact that $W(t)$ is diagonal in the spatial Hilbert space and off diagonal in the spinor space:

$$\langle\varphi_{m,\beta}|W^D(t)|\varphi_{n,\alpha}\rangle = 0, \text{ for } n \neq m, \text{ and } \alpha = \pm,\ \beta = \pm \tag{7}$$

$$\langle\varphi_{n,+}|W^D(t)|\varphi_{n,+}\rangle = \langle\varphi_{n,-}|W^D(t)|\varphi_{n,-}\rangle = 0 \tag{8}$$

$$\langle\varphi_{n,+}|W^D(t)|\varphi_{n,-}\rangle = \langle\varphi_{n,+}|W^D(t)|\varphi_{n,-}\rangle^* = -\frac{qB_x}{m}e^{-i\omega t} \tag{9}$$

$$\to W^D(t) = -\frac{qB_x}{m}\mathbb{I} \otimes \begin{bmatrix} 0 & e^{-i\omega t} \\ e^{i\omega t} & 0 \end{bmatrix} \tag{10}$$

$$\to c_{n,\pm}^{(1)}(t) = \delta_{ni}\left(\delta_{\pm,\alpha} + \frac{i}{\hbar}\frac{qB_x}{m}\int_0^t \mathrm{d}t' e^{\mp i\omega t'}\delta\alpha,\mp\right) = \delta_{ni}\left(\delta_{\pm,\alpha} \mp \frac{i}{\hbar}\frac{qB_x}{m\omega}\left(e^{\mp i\omega t} - 1\right)\delta\alpha,\mp\right) \tag{11}$$

Where the eigenstate was denoted by $|\varphi_{i,+}\rangle$ and the first annullation was obtained by the orthogonality of the spatial parts of the wave-functions, which are left invariant up to a multiplying factor as H_0 is spatial diagonal, so transitions are only allowed to the down spin state but with the same spatial eigenstate.

2. **Diamagnetic susceptibility of the Hydrogen atom**

Determine the diamagnetic susceptibility of the ground state of the hydrogen atom by first order time-independent perturbation theory. Suppose that energy can be written as $E = E_0 + BM$, leading us to the conclusion that $\partial E/\partial B = M$ and $\partial^2 E/\partial B^2 = \chi$. We work in a symmetric gauge:

$$\mathbf{A} = \frac{1}{2}\begin{bmatrix} -By \\ Bx \\ 0 \end{bmatrix} \tag{12}$$

by which the Hamiltonian takes the form:

$$H = \frac{1}{2m}(\mathbf{p} - q\mathbf{A})^2 - \frac{ke^2}{r} = \frac{1}{2m}\left(p_x + \frac{1}{2}qBy\right)^2 + \frac{1}{2m}\left(py - \frac{1}{2}qBx\right)^2 + \frac{1}{2m}p_z^2 - \frac{ke^2}{r} \tag{13}$$

$$H = \frac{\mathbf{p}^2}{2m} + \frac{1}{2}m\left(\frac{\omega_L}{2}\right)^2(x^2 + y^2) - \frac{\omega_L}{2}(xp_y - yp_x) - \frac{ke^2}{r} \tag{14}$$

$$H = \frac{\mathbf{p}^2}{2m} + \frac{1}{2}m\left(\frac{\omega_L}{2}\right)^2(x^2 + y^2) - \frac{\omega_L}{2}L_z - \frac{ke^2}{r} \tag{15}$$

with $\omega_L = \frac{qB}{m}$ the Larmor frequency. In the ground state $l = 0$ we simply have $H_0 = \frac{\mathbf{p}^2}{2m} - \frac{ke^2}{r}$ with perturbation $W = \frac{1}{2}m\left(\frac{\omega_l}{2}\right)^2(x^2 + y^2)$ with the wave function of H_0 $\varphi_{100} = \frac{1}{\sqrt{\pi a_0}}e^{-r/a_0}$. This effective Hamiltonian arises as for $l = 0$ we only have $m = 0$ for which $L_z = 0$!

Now the energy correction induced by the perturbation, writing the perturbation in spherical coordiantes, $W = \frac{m\omega_L^2}{8}\sin^2\theta r^2$

$$\delta E^1(B) = \langle\varphi_{100}|W|\varphi_{100}\rangle = \frac{1}{8}\frac{q^2}{m}B^2\int_0^{2\pi}\mathrm{d}\varphi\int_0^{\pi}\mathrm{d}\theta\int_0^{\infty}\mathrm{d}r\, r^2\frac{1}{\pi a_0^2}e^{-2r/r_0}r^2\sin^3\theta \tag{16}$$

The θ integral gives $\int_{-1}^{1}\mathrm{d}x\, 1 - x^2 = 2 - 2/3 = 4/3$, then the radial integral yields

$$\int_0^{\infty}\mathrm{d}r\, e^{2r/a_0}r^4 = \frac{3a_0^5}{4} \tag{17}$$

yielding altogether for the energy correction $\delta E^{(1)}(B) = \frac{q^2a_0^3}{4m}B^2$, from which the susceptibiltiy reads $\chi = \frac{q^2a_0^3}{2m}$. We can see that we could have dropped from the expectation value of W the $-\frac{\omega_L}{2}L_z$ term for any $l > 0$ quantum number as it is only proportional to $-\frac{\omega_L}{2}L_z \propto B$, giving zeros in the susceptibility. For getting the proper diamagnetic susceptibility contribution from the $-\frac{\omega_L}{2}L_z$ term one should rather consider second order perturbation theory in this term to tget teh coefficient of the quadratic magnetic field term.

3. **Harmonic oscillator in magnetic field:**

The Hamiltonian takes the form:

$$H = \frac{\mathbf{p}^2}{2m} + \frac{1}{2}m\left(\omega^2 + \omega_L^2\right)\left(x^2 + y^2\right) + \frac{1}{2}m\omega^2z^2 - \frac{\omega_L}{2}L_z \tag{18}$$

The z part is already diagonal in terms of the ladder operators, that is they appear as $a_z^\dagger a_z$ in the Hamiltonian while the (x, y) parts needs to be diagonalized as the $L_z = p_x y - p_y x = \frac{ix_0 p_0}{2}\left[\left(a_x^\dagger - a_x\right)\left(a_y^\dagger + a_y\right) - \left(a_y^\dagger - a_y\right)\left(a_x^\dagger + a_x\right)\right] \equiv \frac{i\hbar}{2}\left(a_x^\dagger a_y - a_y^\dagger a_x\right)$

$$H_{xy} = \hbar\Omega\left(a_x^\dagger a_x + a_y^\dagger a_y + 1\right) - i\hbar\frac{\omega_L}{2}\left(a_x^\dagger a_y - a_y^\dagger a_x\right) \tag{19}$$

withe $\Omega^2 = \omega^2 + \omega_L^2$.

Now let us diagonalize the (x, y) part by writing the corresponding Hamiltonian as

$$H_{xy} = \hbar \begin{bmatrix} a_x^\dagger \\ a_y^\dagger \end{bmatrix} \begin{bmatrix} \Omega & i\omega_L/2 \\ -i\omega_L/2 & \Omega \end{bmatrix} \begin{bmatrix} a_x \\ a_y \end{bmatrix} + \hbar\Omega \tag{20}$$

So the task is to diagonalize the matrix connecting the ladder operators of different directions, giving:

$$\begin{bmatrix} \Omega & i\omega_L/2 \\ -i\omega_L/2 & \Omega \end{bmatrix} = \begin{bmatrix} u_{11} & u_{12} \\ u_{21} & u_{22} \end{bmatrix} \begin{bmatrix} \tilde{\omega}_1 & 0 \\ 0 & \tilde{\omega}_2 \end{bmatrix} \begin{bmatrix} u_{11} & u_{21}^* \\ u_{12}^* & u_{22} \end{bmatrix} \tag{21}$$

where the eigenvalues are the new frequencies of the diagonalized Hamiltonian and the u matrix elements determine the roation of the new directions along which we have the new oscillating modes:

$$\tilde{\omega}_{1,2} = \Omega \pm \sqrt{\Omega^2 - \Omega^2 + \omega_L^2/4} = \Omega \pm \omega_L/2 \tag{22}$$

$$\tilde{\omega}_1 = \Omega + \frac{\omega_L}{2}, \ \ \tilde{\omega}_2 = \Omega - \frac{\omega_L}{2} \tag{23}$$

$$\mathbf{u}_1 = \begin{bmatrix} 1 \\ -i \end{bmatrix}, \ \ \mathbf{u}_2 = \begin{bmatrix} 1 \\ i \end{bmatrix} \tag{24}$$

$$\Rightarrow H_{xy} = \hbar \begin{bmatrix} a_x^\dagger \\ a_y^\dagger \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} \\ u_{21} & u_{22} \end{bmatrix} \begin{bmatrix} \tilde{\omega}_1 & 0 \\ 0 & \tilde{\omega}_2 \end{bmatrix} \begin{bmatrix} u_{11} & u_{21}^* \\ u_{12}^* & u_{22} \end{bmatrix} \begin{bmatrix} a_x \\ a_y \end{bmatrix} = \hbar \begin{bmatrix} \mathbf{a}\cdot\mathbf{u}_1 \\ \mathbf{a}\cdot\mathbf{u}_2 \end{bmatrix} \begin{bmatrix} \tilde{\omega}_1 & 0 \\ 0 & \tilde{\omega}_2 \end{bmatrix} \begin{bmatrix} \mathbf{a}\cdot\mathbf{u}_1^* \\ \mathbf{a}\cdot\mathbf{u}_2^* \end{bmatrix} + \hbar\Omega \tag{25}$$

$$\tilde{a}_1 = a_x + i a_y, \ \ \tilde{a}_2 = a_x - i a_y \tag{26}$$

yielding the digaonal total Hamiltonian:

$$H = \hbar\tilde{\omega}_1 \tilde{a}_1^\dagger \tilde{a}_1 + \hbar\tilde{\omega}_2 \tilde{a}_2^\dagger \tilde{a}_2 + \hbar\omega\left(a_z^\dagger a_z + \frac{1}{2}\right) + \hbar\Omega \tag{27}$$

So the energy spectrum is

$$E_{nml} = \hbar\tilde{\omega}_1 n + \hbar\tilde{\omega}_2 m + \hbar\omega\left(l + \frac{1}{2}\right) + \hbar\Omega \tag{28}$$

This is similar to the so called Bogolyubov transformation, common in e.g.: superconductivity or low temeprature Bose-Einstein condensates.

Note further that here we have infinitely many degeneracies FOR $\omega = 0$ with energies $E_{nm} = \hbar\frac{\omega_L}{2}(n - m) + \hbar\omega_L \Rightarrow E_{nn} = \hbar\omega_L \, \forall n$.