Kvantmehaanika, loengud 14–16

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2. **Write the general Schrodinger equation for perturbation theory in degenerate case. Helping parameter.**

Writing energy operator as:

$$\hat{H} = \hat{H}_0 + \lambda \hat{H}'$$

where λ is the helping parameter (after solving $\lambda = 0$). Expanding the energy and state in powers of λ:

$$E_n = E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \dots,$$
$$\psi_n = \psi_n^0 + \lambda \psi_n^1 + \lambda^2 \psi_n^2 + \dots.$$

Equating the terms:

$$\left(\hat{H}_0 + \lambda \hat{H}'\right)\left(\psi_n^0 + \lambda\psi_n^1 + \lambda^2\psi_n^2 + \dots\right) = \left(E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \dots\right)\left(\psi_n^0 + \lambda\psi_n^1 + \lambda^2\psi_n^2 + \dots\right)$$

Written as a system:

$$\begin{aligned} \lambda^0: &\quad \hat{H}_0\psi_n^0 = E_n^0\psi_n^0 \\ \lambda^1: &\quad \hat{H}_0\psi_n^1 + \hat{H}'\psi_n^0 = E_n^0\psi_n^1 + E_n^1\psi_n^0 \\ \lambda^2: &\quad \hat{H}_0\psi_n^2 + \hat{H}'\psi_n^1 = E_n^0\psi_n^2 + E_n^1\psi_n^1 + E_n^2\psi_n^0 \\ &\dots \end{aligned}$$

For a degenerate level E_n^0, choosing an orthonormal basis $\{\psi_{n,i}^0\}_{i=1}^r$ satisfying $\hat{H}_0\,\psi_{n,i}^0 = E_n^0\,\psi_{n,i}^0$. Introducing matrix elements:

$$H'_{ij} = \int \psi_{ni} * \hat{H}'\psi_{nj} dV = \langle \psi_{n,i}^0 | \hat{H}' | \psi_{n,j}^0 \rangle.$$

Giving:

$$\sum_{j=1}^{r} \left(E_n^1 \delta_{ij} - H'_{ij}\right) c_j = 0, \quad i = 1, 2, \dots, r$$

Written as a matrix:

$$\begin{pmatrix} E_n^1 - H'_{11} & -H'_{12} & \cdots & -H'_{1r} \\ -H'_{21} & E_n^1 - H'_{22} & \cdots & -H'_{2r} \\ \vdots & \vdots & \ddots & \vdots \\ -H'_{r1} & -H'_{r2} & \cdots & E_n^1 - H'_{rr} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_r \end{pmatrix} = 0.$$

$$\begin{vmatrix} E_n^1 - H'{}_{11} & -H'_{12} & \cdots & -H'_{1r} \\ -H'_{21} & E_n^1 - H'_{22} & \cdots & -H'_{2r} \\ \vdots & \vdots & \ddots & \vdots \\ -H'_{r1} & -H'_{r2} & \cdots & E_n^1 - H'_{rr} \end{vmatrix} = 0.$$

If the determinant is zero, there are nontrivial solutions c_j. The corresponding eigenvectors c_j^i define the corrected zeroth-order states as:

$$\psi_n^i = \sum_{j=1}^{r} c_j^i \psi_{nj}$$

11. **Calculation the probability of interlevel transition for harmonic oscillator and hydrogen atom in external electromagnetic wave by using "golden rule". Selecton rules. (vt. Loide raamat lk.120 §22.)**

Considering a system (harmonic oscillator or hydrogen atom) subject to an electric field:

$$\mathbf{E}(t) = E_0 \cos\omega t\, \hat{z}$$

in the electric–dipole approximation ($\mathbf{k}\cdot\mathbf{r} \approx 0$). The time-dependent perturbation Hamiltonian:

$$\hat{H}'(t) \;=\; -e\,\mathbf{r}\cdot\mathbf{E}_0 \cos\omega t \;=\; -e\,z\,E_0 \cos\omega t \;=\; \tfrac{1}{2}\big(h\,e^{-i\omega t} + h^\dagger\,e^{+i\omega t}\big),$$

where

$$h_{mn} \;=\; \langle m|h|n\rangle \;=\; -\,eE_0 \underbrace{\int \psi_m^*(\mathbf{r})\,z\,\psi_n(\mathbf{r})\,d^3r}_{z_{mn}}.$$

"Golden rule"then gives the induced transition probability per unit time:

$$\frac{dP_{nm}}{dt} = \frac{2\pi}{\hbar}\,\big|h_{mn}\big|^2\,\delta\big(E_m - E_n \pm \hbar\omega\big) = \frac{2\pi}{\hbar}\,e^2E_0^2\,\big|z_{mn}\big|^2\,\delta\big(E_m - E_n \pm \hbar\omega\big).$$

At resonance $\omega = \omega_{mn} = (E_m - E_n)/\hbar$:

$$\frac{dP_{mn}}{dt} = \frac{\pi\,e^2E_0^2}{\hbar^2}\,\big|z_{mn}\big|^2.$$

Harmonic oscillator

For a harmonic oscillator, the only nonzero dipole matrix elements:

$$\langle n\pm 1|x|n\rangle = \sqrt{\frac{\hbar}{2m\omega_0}}\begin{cases}\sqrt{n+1}, & \text{if } m = n+1,\\ \sqrt{n}, & \text{if } m = n-1,\\ 0, & \text{otherwise.}\end{cases}$$

$$h_{n,n\pm 1} = -eE_0\,\langle n\pm 1|x|n\rangle \neq 0 \implies \Delta n = \pm 1.$$

All other transitions are forbidden. Thus the allowed processes:

$$n \to n+1 \text{ (absorption, } \Delta n = +1), \qquad n \to n-1 \text{ (emission, } \Delta n = -1).$$

Hydrogen atom

The stationary states in a hydrogen atom:

$$|n\,l\,m\,\sigma\rangle = \psi_{nlm}(r,\theta,\varphi)\;Y_{1/2\,\sigma}, \quad |n'\,l'\,m'\,\sigma'\rangle = \psi_{n'l'm'}(r,\theta,\varphi)\;Y_{1/2\,\sigma'}.$$

Here $\psi_{nlm}(r,\theta,\varphi) = R_{nl}(r)\,Y_{lm}(\theta,\varphi)$ and $dV = r^2\,dr\,d\Omega$. The spatial matrix elements separate into a radial and an angular part:

$$x_{ij} = \delta_{\sigma'\sigma}\int \psi_{n'l'm'}^*(\mathbf{r})\,x\,\psi_{nlm}(\mathbf{r})\,dV = \delta_{\sigma'\sigma}\int_0^\infty r^3 R_{n'l'}(r)R_{nl}(r)\,dr \int Y_{l'm'}^*\,\sin\theta\cos\varphi\,Y_{lm}\,d\Omega.$$

and similarly for y_{ij} and z_{ij} with $\sin\theta\sin\varphi$ and $\cos\theta$ respectively. Using the spherical-harmonic identities

$$\sin\theta\cos\varphi = \sqrt{\tfrac{2\pi}{3}}\big(Y_{1,-1} - Y_{1,1}\big), \quad \sin\theta\sin\varphi = i\sqrt{\tfrac{2\pi}{3}}\big(Y_{1,-1} + Y_{1,1}\big), \quad \cos\theta = \sqrt{\tfrac{4\pi}{3}}\,Y_{1,0},$$

one finds that the angular integrals are nonzero only for

$$\Delta l = l' - l = \pm 1, \qquad \Delta m = m' - m = 0, \pm 1,$$

recovering the electric-dipole selection rules as above. The remaining radial integral

$$I_{nl,n'l'} = \int_0^\infty R_{n'l'}(r)\,r^3\,R_{nl}(r)\,dr$$

determines the overall transition strength. Transitions with $\Delta m = 0$ produce radiation linearly polarized along z, while $\Delta m = \pm 1$ produce circular polarization in the xy-plane.

13. **What is the meaning of the theorem on the relationship between spin and statistics?**

In quantum mechanics the intrinsic spin of a particle (angular momentum not due to orbital motion) determines the symmetry of its many-particle wavefunction and hence the statistics it obeys:

- **Bosons:** $s \in \{0, 1, 2, \dots\}$ (integer spin). The particle wavefunction is symmetric under exchange of any two particles. Any number of bosons may occupy the same quantum state. The probability of finding a particle in a state with energy E is given by the Bose–Einstein distribution:
$$f(E, T) \; = \; \frac{1}{e^{E/kT} - 1} \, .$$
Examples: photons, phonons.

- **Fermions:** $s \in \{\frac{1}{2}, \frac{3}{2}, \dots\}$ (half-integer spin). The particle wavefunction is antisymmetric under exchange of any two particles, enforcing the Pauli exclusion principle: only one fermion perquantum state. The probability of finding a particle in a state with energy E is given by the Fermi–Dirac distribution:
$$f(E, T) \; = \; \frac{1}{e^{(E-\mu)/kT} + 1} \, ,$$
where mu is chemical potential. For metals at room temperature the chemical potential can be replaced by the Fermi energy. **Examples:** proton, neutron, electron.