

Kvantmehaanika, loengud 10–13

Ivan Novoseltsev, 233137YAFB

20

7. **Is it possible measure simultaneously absolute value of angular momentum $|\vec{L}|$ and its x projection? Why? Proof.**

Yes. The operators $\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$, \hat{L}_x commute:

$$[\hat{L}^2, \hat{L}_x] = [\hat{L}_x^2, \hat{L}_x] + [\hat{L}_y^2, \hat{L}_x] + [\hat{L}_z^2, \hat{L}_x].$$

Since $[\hat{L}_x^2, \hat{L}_x] = 0$ and using commutation relations $[\hat{L}_y, \hat{L}_x] = i\hbar \hat{L}_z$, $[\hat{L}_z, \hat{L}_x] = -i\hbar \hat{L}_y$:

$$\begin{aligned} [\hat{L}_y^2, \hat{L}_x] &= \hat{L}_y[\hat{L}_y, \hat{L}_x] + [\hat{L}_y, \hat{L}_x]\hat{L}_y = i\hbar (\hat{L}_y \hat{L}_z + \hat{L}_z \hat{L}_y), \\ [\hat{L}_z^2, \hat{L}_x] &= \hat{L}_z[\hat{L}_z, \hat{L}_x] + [\hat{L}_z, \hat{L}_x]\hat{L}_z = -i\hbar (\hat{L}_z \hat{L}_y + \hat{L}_y \hat{L}_z), \end{aligned}$$

so that $[\hat{L}_y^2, \hat{L}_x] + [\hat{L}_z^2, \hat{L}_x] = 0$ and hence $[\hat{L}^2, \hat{L}_x] = 0$. Commuting observables have a common eigenbasis $\{|l, m_x\rangle\}$ with $\hat{L}^2|l, m_x\rangle = \hbar^2 l(l+1)|l, m_x\rangle$ and $\hat{L}_x|l, m_x\rangle = \hbar m_x|l, m_x\rangle$, so $L = |\vec{L}|$ and L_x can be measured simultaneously.

13. **Write an expression for the x , y and z projection of the angular frequency operators $\hat{\omega}_x$, $\hat{\omega}_y$, and $\hat{\omega}_z$ (the rotating body is a homogeneous sphere of mass M and radius R).**

In classical mechanics, the angular momentum vector \vec{L} of a rigid body is related to its angular velocity $\vec{\omega}$ by the inertia tensor \vec{I} :

$$\vec{L} = \vec{I}\vec{\omega}.$$

For a homogeneous sphere the inertia tensor becomes scalar,

$$\begin{aligned} I &= \int_V (r \sin \theta)^2 \rho r^2 \sin \theta dr d\theta d\phi = \rho \int_0^R \int_0^\pi \int_0^{2\pi} r^4 \sin^3 \theta d\phi d\theta dr = \\ &= \underbrace{\rho}_{=M/V} \cdot 2\pi \cdot 4/3 \cdot R^5/5 = \frac{3M \cdot 2\pi \cdot 4 \cdot R^5}{4\pi R^3 \cdot 3 \cdot 5} = \frac{2}{5} MR^2, \end{aligned}$$

so that $\hat{\vec{L}} = I \hat{\vec{\omega}}$. In quantum mechanics, the corresponding classical quantities are represented by operators: $\hat{\vec{L}} = (\hat{L}_x, \hat{L}_y, \hat{L}_z)$ and $\hat{\vec{\omega}} = (\hat{\omega}_x, \hat{\omega}_y, \hat{\omega}_z)$. Since $\vec{I} = I \vec{1}$, it follows that $\hat{\vec{\omega}} = \frac{\hat{\vec{L}}}{I}$. Hence, each component of the angular velocity operator is proportional to the corresponding component of the angular momentum operator:

$$\hat{\omega}_x = \frac{\hat{L}_x}{I}, \quad \hat{\omega}_y = \frac{\hat{L}_y}{I}, \quad \hat{\omega}_z = \frac{\hat{L}_z}{I}.$$

20. **Obtain the equation for radial part of wave function:**

$$-\frac{\hbar^2}{2M} \left[\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dR(r)}{dr} \right) \right] + \left[\frac{\hbar^2 l(l+1)}{2M r^2} + U(r) \right] R_{nl}(r) = E R_{nl}(r),$$

Starting from the time-independent Schrödinger equation:

$$-\frac{\hbar^2}{2M} \nabla^2 \psi(\vec{r}) + U(r) \psi(\vec{r}) = E \psi(\vec{r}).$$

In spherical coordinates:

$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) - \frac{1}{r^2} \hat{L}_{\theta\phi}^2.$$

Separating the variables:

$$\psi_{n\ell m}(r, \theta, \phi) = R_{n\ell}(r) Y_{\ell m}(\theta, \phi),$$

where $Y_{\ell m}$ are spherical harmonics and $R_{n\ell}(r)$ is purely radial. Substituting into the full equation:

$$-\frac{\hbar^2}{2M} \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) - \frac{1}{r^2} \hat{L}_{\theta\phi}^2(RY) \right] + U(r) RY = E RY.$$

Separating radial and angular parts:

$$\frac{\partial}{\partial r} = Y R', \quad \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) = Y \frac{d}{dr} (r^2 R'),$$

and $\hat{L}_{\theta\phi}^2(RY) = R \hat{L}_{\theta\phi}^2 Y$. Using the eigenvalue equation for spherical harmonics:

$$\hat{L}_{\theta\phi}^2 Y_{\ell m} = \hbar^2 \ell(\ell+1) Y_{\ell m}, \quad \text{so } \hat{L}_{\theta\phi}^2(RY) = \hbar^2 \ell(\ell+1) RY.$$

Substituting and dividing by Y :

$$-\frac{\hbar^2}{2M} \left[\frac{1}{r^2} \frac{d}{dr} (r^2 R') - \frac{\ell(\ell+1)}{r^2} R \right] + U(r) R = E R.$$

Rearranging to the standard form:

$$-\frac{\hbar^2}{2M} \left[\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) \right] + \left[\frac{\hbar^2 \ell(\ell+1)}{2M r^2} + U(r) \right] R(r) = E R(r).$$

36. How looks like the electron configuration for Li, Na and K atoms? Why? What do all these materials have in common (in terms of physical properties)? How does this relate to the configuration of the electrons?

- **Lithium (Li, $Z = 3$):** $1s^2 2s^1$.
- **Sodium (Na, $Z = 11$):** $1s^2 2s^2 2p^6 3s^1$.
- **Potassium (K, $Z = 19$):** $1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$.

18

Reasons:

- Principle of minimum energy. Electrons fill orbitals in order of increasing energy: $E_{1s} < E_{2s} < E_{2p} < E_{3s} < \dots$
- Exclusion principle. Each spatial orbital, specified by the quantum numbers, can accommodate at most two electrons, and these two must have opposite spin quantum numbers: $m_s = +\frac{1}{2}$ and $m_s = -\frac{1}{2}$.
- Screening and effective nuclear charge. Core electrons generate a spherically symmetric potential that partially screens the nuclear charge. As a result, the valence electron experiences an effective charge Z_{eff} and moves in a central potential whose energy levels follow the same ordering derived from the radial Schrödinger equation.

From this it follows that an electron will occupy the first available (lowest-energy) s -orbital of principal quantum number n , yielding the configuration ns^1 .

Consequences (because of the common valence configuration ns^1):

- Low first ionization energy: the lone s -electron is only weakly bound.
- Formation of M^+ cations: they readily lose one electron.
- Characteristic group-1 ("alkali metal") properties: high chemical reactivity, metallic luster, softness, low melting points and high electrical conductivity.

45. Why for the second-order energy correction of a harmonic oscillator in a constant force field (p. 129) we need to take into account only two terms of the sum n , $n+1$ and n , $n-1$.

The perturbation by a constant force F is

$$\hat{H}' = F \hat{x}.$$

10

Expressing the position operator in terms of creation and annihilation operators:

$$\hat{x} = \sqrt{\frac{\hbar}{2M\omega}} (a + a^\dagger).$$

The perturbation matrix has nonzero elements only between adjacent levels:

$$\langle k | \hat{H}' | n \rangle = F \sqrt{\frac{\hbar}{2M\omega}} (\langle k | a | n \rangle + \langle k | a^\dagger | n \rangle)$$

Since

$$a | n \rangle = \sqrt{n} | n - 1 \rangle, \quad a^\dagger | n \rangle = \sqrt{n + 1} | n + 1 \rangle,$$

It follows that

$$\langle k | \hat{H}' | n \rangle \neq 0 \implies k = n \pm 1.$$

follows from what?

Therefore, the second-order correction

$$E_n^{(2)} = \sum_{k \neq n} \frac{|\langle k | \hat{H}' | n \rangle|^2}{E_n^{(0)} - E_k^{(0)}} = \frac{|\langle n - 1 | \hat{H}' | n \rangle|^2}{E_n^{(0)} - E_{n-1}^{(0)}} + \frac{|\langle n + 1 | \hat{H}' | n \rangle|^2}{E_n^{(0)} - E_{n+1}^{(0)}}.$$

thus contains contributions only from $k = n + 1$ and $k = n - 1$, since for all other k the numerator vanishes.