Homework to exercise 14

Exam preparation

Send the solutions to 2.and 3. to your seminar leader by january 30th 2024

1. When preparing to tasks 2-6 of the exam, it is recommended to repeat:

- Dielectric function and optical constants
- Momentum and energy conservation in collision events (relativistic and non-relativistic approaches)
- Properties of linear operators
- Commutation relations
- Expectation values
- Spherical coordinates and hydrogen atom
- Vibrations of molecules

2. Multiple-choice test: Please tick all box(es) with correct answer(s)!
(correctly ticked box: +1/2 point; wrongly ticked box: -1/2 point)

The rule of mutual exclusion in Raman spectroscopy	Concerns centrosymmetric systems	✓
	Forbids any Raman-activity in organic molecules	
	Is only valid in metals	
The operator of discrete translations $\hat{\mathbf{T}}_n$ defined by: $\hat{\mathbf{T}}_n \psi(\mathbf{r}) = \psi(\mathbf{r}+\mathbf{r}_n)$	is self-adjoint	
	is not self-adjoint	✓

3. Imagine a non-relativistic hydrogen atom in the excited quantum state $|n,l,m\rangle = |2,1,1\rangle$. In spherical coordinates, the wavefunction of the electron in that state may be written as:

$$\psi(r,\varphi,\theta) = \frac{1}{8\sqrt{\pi}}\left(\frac{1}{a_0}\right)^{\frac{3}{2}} \frac{r}{a_0} e^{-\frac{r}{2a_0}} \sin\theta e^{i\varphi}$$

. a_0 is the Bohr's radius. Calculate the expectation value $\langle r \rangle$ as well as the variance $\mathrm{var}(r) = \langle r^2 \rangle - \langle r \rangle^2$ of r in this quantum state!
(10 points)

$$\langle r \rangle = \int_V \psi^* r \psi \, dV = \iiint r \psi \cdot \psi^* r^2 \sin\theta \, dr \, d\theta \, d\varphi$$

$$= \iiint \frac{1}{64\pi}\left(\frac{1}{a_0}\right)^3 \frac{r^2}{a_0^2} e^{-\frac{r}{a_0}} \cdot r^3 \sin^3\theta \, dr \, d\theta \, d\varphi =$$

$$= \frac{1}{64\pi a_0^5} \int_0^{2\pi} d\varphi \int_0^{\pi} \sin^3\theta \, d\theta \int_0^{\infty} r^5 e^{-\frac{r}{a_0}} dr = \frac{2\pi}{64\pi a_0^5} \cdot \frac{5!}{\left(\frac{1}{a_0}\right)^6} \int_0^{\pi} \sin^3\theta \, d\theta$$

$$= \frac{a_0 5!}{32} \cdot \frac{4}{3} = 5a_0$$

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$$\langle r^2\rangle = \int_V \psi^* r^2 \psi \, dV = \iiint \frac{1}{64\pi}\left(\frac{1}{a_0}\right)^3 \frac{r^2}{a_0^2} e^{-\frac{r}{a_0}} \sin^2\theta \cdot r^2 \cdot r^2 \sin\theta \, dr$$

$$= \frac{1}{64\pi a_0^5} \int_0^{2\pi} d\varphi \int_0^{\pi} \sin^3\theta \, d\theta \int r^6 e^{-\frac{r}{a_0}} dr$$

$$= \frac{1}{64\pi a_0^5} \cdot 2\pi \cdot \frac{4}{3} \cdot \frac{6!}{\left(\frac{1}{a_0}\right)^7} = 30 a_0^2$$

$$\mathrm{Var}\langle r\rangle = \langle r^2\rangle - \langle r\rangle^2 = 5a_0^2$$

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