

Quantenmechanik, Herbstsemester 2021

Blatt 8

Abgabe: 16.11.21, 12:00H (Treppenhaus 4. Stock)

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- (1) **Isotropic 3-dimensional harmonic oscillator** (3 Punkte)
Consider the isotropic 3-dimensional harmonic oscillator defined by the Hamiltonian

$$H = \frac{1}{2m} \sum_{i \in \{x,y,z\}} p_i^2 + \frac{1}{2} m \omega^2 \sum_{i \in \{x,y,z\}} x_i^2.$$

As usual when dealing with spherically symmetric potentials we split the wavefunction in radial and angular parts and write

$$\Psi_{Elm} = \frac{u_{El}(r)}{r} Y_{lm}(\theta, \phi),$$

and obtain the Schrödinger equation for the radial part

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + \frac{1}{2} m \omega^2 r^2 + \frac{\hbar^2}{2m} \frac{l(l+1)}{r^2} - E \right] u(r) = 0,$$

where the (E, l) -dependence of $u(r)$ has been omitted.

- (a) Using the ansatz wavefunction

$$u(r) = e^{-y^2/2} v(y), \quad y = r \sqrt{m\omega/\hbar},$$

to derive a differential equation for $v(y)$.

What is the boundary condition on $v(y)$ for $y = 0$?

Result: $v''(y) - 2yv'(y) + [2\lambda - 1 - l(l+1)/y^2]v(y) = 0$ where $\lambda = E/(\hbar\omega)$.

- (b) To further investigate the differential equation obtained in (a), we expand $v(y)$ as

$$v(y) = y^{l+1} \sum_{j=0}^{\infty} C_j y^j. \quad (1)$$

Explain the factor r^{l+1} . Derive a two-term recursion relation for the coefficients C_j , i.e., an equation relating C_j and C_{j+2} . Hint: show that $C_1 = 0$.

- (c) Find the energy eigenvalues by using the two-term recursion relation and the requirement that the series (1) has to converge for $r \rightarrow \infty$.
- (d) Compare the result from (c) with the energy quantization found when using second quantized operators, i.e., $H = \hbar\omega \sum_{i \in \{x,y,z\}} (a_i^\dagger a_i + \frac{1}{2})$, which was discussed in the lecture.

Show explicitly that both methods give the same (i) quantization of the energy, and (ii) degeneracy of the levels.

(2) **Hydrogen atom in $n = 2, l = 1$ state** (3 Punkte)

Assume that the electron in a hydrogen atom occupies the following combined spin and position eigenstate

$$\psi(r, \theta, \phi) = R_{21}(r) \left(\sqrt{\frac{1}{3}} Y_{10}(\theta, \phi) |\uparrow\rangle + \sqrt{\frac{2}{3}} Y_{11}(\theta, \phi) |\downarrow\rangle \right).$$

- (a) What are the possible measurement results if you measure the z -component of angular momentum L_z , and what is the probability of each?
- (b) Same for the z -component of spin angular momentum S_z .
- (c) Let $\mathbf{J} = \mathbf{L} + \mathbf{S}$ be the total angular momentum. If you measure J^2 , what are the possible measurement results, and what is the probability of each?
Hint: Use the Clebsch-Gordan table.
- (d) If you measure the position of the electron, what is the probability of finding it at r, θ, ϕ ? Hint: $R_{21}(r) = \frac{1}{2\sqrt{6}} a^{-3/2} \left(\frac{r}{a}\right) \exp(-r/(2a))$ where a is the Bohr radius.

(3) **Coupled spins** (2 Punkte + 2 Bonuspunkte)

Consider two coupled spin 1/2 particles in an external magnetic field $\mathbf{B} = (0, 0, B)$ along the z -direction, with the Hamiltonian

$$H = J \mathbf{S}_1 \cdot \mathbf{S}_2 - \frac{\mu}{\hbar} B (S_{1z} + S_{2z}),$$

where $J > 0$. Determine and discuss the energy eigenvalues and eigenstates. Plot the energies of the ground state and of the excited states as a function of the magnetic field B .

Hint: Consider $\mathbf{S} = \mathbf{S}_1 + \mathbf{S}_2$ and express the Hamiltonian in terms of $S^2, S_1^2,$ and S_2^2 .

Bonus points: Same for three spins arranged on the corners of a triangle. This situation is called “geometrically frustrated”, can you imagine why? Use a computer for $B \neq 0$.

(4) **Variational method** (2 Punkte + 2 Bonuspunkte)

- (a) Use the variational ansatz $\psi_\lambda(x) \propto \exp(-\frac{x^2}{2\lambda^2})$ to show that the one-dimensional potential well

$$V(x) = \begin{cases} -V_0 & |x| < a, \\ 0 & |x| \geq a \end{cases}$$

with $V_0 > 0$ has *at least* one bound state.

Hint: Show that it is possible to find a negative upper bound for the ground-state energy.

Bonus points: Show that the existence of a bound state is *not* guaranteed in the three-dimensional case. And what about the two-dimensional case?

- (b) Find an upper bound for the ground-state energy of the Hamiltonian

$$H = \frac{p^2}{2m} + kx^4, \quad k > 0,$$

by choosing an appropriate trial wavefunction.

Compare with the exact result

$$E_0 = 0.66798626 \dots \left(\frac{\hbar^4 k}{m^2} \right)^{1/3}.$$