Hamiltonian

$$\hat{H} = \hat{p}^2/2m + V(x)$$

Harmonic oscillator

$$\begin{aligned} V(x) &= \frac{1}{2}m\omega^2 x^2 \\ \psi_n(x) &= A_n(a^+)^n \psi_0(x) \\ E_n &= (n+\frac{1}{2})\hbar\omega \\ \hat{x} &= \sqrt{\frac{\hbar}{2m\omega}}(\hat{a}^+ + \hat{a}^-) \\ \hat{p} &= i\sqrt{\frac{\hbar m\omega}{2}}(\hat{a}^+ - \hat{a}^-) \end{aligned}$$

Wavefunctions

$$\begin{aligned} \psi_n(x) &= \frac{1}{\sqrt{2^n\, n!}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\xi^2/2} H_n(\xi) \\ \xi &= (m\omega/\hbar)^{1/2} x \\ H_0(x) &= 1;\ H_1(x) = 2x, \\ H_2(x) &= 4x^2 - 2, \\ H_3(x) &= 8x^3 - 12x, \\ H_4(x) &= 16x^4 - 48x^2 + 12 \end{aligned}$$

Gaussian integrals

$$\int_0^\infty x^{2n} e^{-\frac{x^2}{a^2}}\, dx = \sqrt{\pi}\frac{a^{2n+1}(2n)!}{2^{2n+1}n!}$$

$$\int_0^\infty x^{2n+1} e^{-\frac{x^2}{a^2}}\, dx = \frac{n!}{2}a^{2n+2}$$

Bohr radius

$$a = \frac{4\pi\varepsilon_0\hbar^2}{me^2}$$

Fourier transforms

$$\begin{aligned} f(x) &= (2\pi)^{-1/2}\int_{-\infty}^{\infty} F(k)e^{ikx}dk \\ F(k) &= (2\pi)^{-1/2}\int_{-\infty}^{\infty} f(x)e^{-ikx}dx \\ \phi(k) &= (2\pi)^{-1/2}\int_{-\infty}^{\infty} \Psi(x,0)e^{-ikx}dx \end{aligned}$$

Time evolution of a free particle

$$\Psi(x,t) = (2\pi)^{-1/2}\int_{-\infty}^{\infty}\phi(k)e^{ikx - i(\hbar k^2/2m)t}dk$$

Phase and group velocity

$$\begin{aligned} v_\phi &= \omega/k \\ v_g &= d\omega/dk \end{aligned}$$

Jump in derivative at potential $-\alpha\delta(x)$

$$\Delta(\frac{d\psi}{dx}) = -\frac{2m\alpha}{\hbar^2}\psi(0)$$

Probability current

$$J = \frac{i\hbar}{2m}\left(\Psi\frac{\partial\Psi^*}{\partial x} - \Psi^*\frac{\partial\Psi}{\partial x}\right)$$

Trigonometry

$$\begin{aligned} \sin(A \pm B) &= \sin A\cos B \pm \cos A \sin B \\ \cos(A \pm B) &= \cos A\cos B \mp \sin A \sin B \end{aligned}$$

Hamiltonian of an atom

$$\begin{aligned} H &= \sum_{i=1}^{Z}\left(-\frac{\hbar^2}{2\mu}\nabla^2_{r_i} - \frac{Ze^2}{4\pi\epsilon_0 r_i}\right) \\ &+ \sum_{i<j}^{Z}\frac{e^2}{4\pi\epsilon_0 r_{ij}} \end{aligned}$$

Ground state of H

$$\psi_{100} = \frac{1}{\sqrt{\pi a^3}}e^{-r/a};\ E_1 = \frac{-m}{2\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2$$

Angular momentum ladder operators

$$\begin{aligned} L_\pm &= L_x \pm iL_y \\ L_\pm|l,m\rangle &= \hbar\sqrt{l(l+1) - m(m\pm 1)}|l, m\pm 1\rangle \end{aligned}$$

Angular momentum

$$\begin{aligned} \mathbf{L} &= -i\hbar\mathbf{r}\times\nabla \\ L_z &= -i\hbar\frac{\partial}{\partial\phi} \end{aligned}$$

Angular momentum algebra

$$[L_x, L_y] = i\hbar L_z \qquad \text{and cyclic perm.}$$

Eigenvalues of angular momentum

$$\begin{aligned} L^2 Y_\ell^m(\theta,\phi) &= \hbar^2 \ell(\ell+1) Y_\ell^m(\theta,\phi); \\ L_z Y_\ell^m &= \hbar m Y_\ell^m; \\ Y_\ell^m(\theta,\phi) &\propto e^{im\phi} P_\ell^m(\cos\theta) \end{aligned}$$

Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Coupling angular momentum

$$\begin{aligned} j &= (j_1 + j_2), (j_1 + j_2 - 1), \ldots, |j_1 - j_2| \\ m_j &= -j, -j+1, \ldots j-1, j \end{aligned}$$

Bose/Fermi symmetric two-paricle states

$$\Psi_\pm(x_1, x_2, s_1, s_2) = \frac{\Psi_1(x_1, s_1)\Psi_2(x_2, s_2) \pm \Psi_2(x_1, s_1)\Psi_1(x_2, s_2)}{\sqrt{2}}$$

Laplacian

$$\begin{aligned} \nabla^2 &= \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta \frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\varphi^2} \\ &= \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) - \frac{1}{\hbar^2 r^2} L^2 \end{aligned}$$

Radial equation

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \left[V + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}\right] u = Eu$$

Solutions for the spherical infinite well

$$\psi_{nlm} = A_{nl} j_l(\beta_{nl} r/a) Y_l^m(\theta,\phi)$$

Fermi energy

$$E_F = \frac{\hbar^2}{2m}(3\pi^2 N_e/V)^{2/3}$$

Perturbation of the wavefunction

$$\psi_n^1 = \sum_{m\neq n} \frac{\langle \psi_m^0 | H' | \psi_n^0 \rangle}{E_n^0 - E_m^0} \psi_m^0$$

Second order perturbation of the energy

$$E_n^2 = \sum_{m\neq n} \frac{|\langle \psi_m^0 | H' | \psi_n^0 \rangle|^2}{E_n^0 - E_m^0}$$

Rydberg wavelength formula

$$\lambda^{-1} = \frac{m}{4\pi c\hbar^3}\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2 (n_f^{-2} - n_i^{-2})$$

Bohr energy

$$E_1 = -\frac{m_e}{2\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2$$

Time derivative of an expectation value

$$\frac{d}{dt}\langle Q \rangle = \frac{i}{\hbar}\langle [\hat{H}, \hat{Q}] \rangle + \langle \frac{\partial Q}{\partial t} \rangle$$

Virial theorem

$$2\langle T \rangle = \langle x \frac{dV}{dx} \rangle$$

Generalized uncertainty principle

$$\sigma_A^2 \sigma_B^2 \geq \left(\frac{1}{2i}\langle [\hat{A}, \hat{B}] \rangle\right)^2$$

Commutator identity

$$[AB, C] = A[B, C] + [A, C]B$$

Hermitian conjugate

$$\langle f, \hat{Q} g \rangle = \langle \hat{Q}^\dagger f, g \rangle \ \forall f, g$$

Translation operator

$$\hat{T}(\mathbf{x}) = \exp\left(-\frac{i\mathbf{x}\cdot\hat{\mathbf{p}}}{\hbar}\right)$$

Transformation of an operator

$$\hat{Q}' = \hat{T}^\dagger \hat{Q} \hat{T}$$

Rotation operator

$$\hat{R}(\mathbf{n}, \phi) = \exp\left(-\frac{i\phi}{\hbar}\mathbf{n}\cdot\hat{\mathbf{L}}\right)$$

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You may use no other materials than pen, paper, drawing tools and the formula sheet included with this test. A (graphical) calculator is allowed unless it can transmit or receive signals. The regular time for this test is **180** minutes. This test has **17** questions on **6** pages, for a total of **30** points.

Motivate all your answers, using words, calculations or drawings. Stating only the final answer without motivation will not be awarded points. You may answer in Dutch or English. Unclear and unreadable answers will be considered wrong.

Please use a new sheet of answer paper for each of the three sections. Write your NAME and STUDENT NUMBER on every answer sheet. Success!

1 Larmor precession (6 points)

We consider a spin $S = 1/2$ system in a magnetic field in x-direction. The Hamiltonian is given by

$$H = \frac{-\mu B}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tag{1}$$

where μ is the magnetic moment, B the strength of the magnetic field, and both are positive.

a. (1 point) Verify that H has the eigenvalues $E_{\pm} = \pm\frac{\mu B}{2}$,

b. (1 point) and that the corresponding eigenvectors are $|+\rangle = \frac{1}{\sqrt{2}}(1,-1)^T$ and $|-\rangle = \frac{1}{\sqrt{2}}(1,1)^T$.

We now want to study the time evolution of a quantum state. At time $t = 0$, it was initialized as a spin down, *i.e.*,

$$|\psi(t=0)\rangle = |\downarrow\rangle = (0,1)^T.$$

The time evolution is dictated by the time-dependent Schrödinger equation with the solution

$$|\psi(t)\rangle = e^{-i\frac{H}{\hbar}t}|\psi(t=0)\rangle.$$

c. (1 point) Express $|\psi(t=0)\rangle$ in terms of $|+\rangle$ and $|-\rangle$.

d. (2 points) Show that its time evolution is given by $|\psi(t)\rangle = -\frac{1}{\sqrt{2}}e^{-i\frac{\mu B}{2\hbar}t}|+\rangle + \frac{1}{\sqrt{2}}e^{i\frac{\mu B}{2\hbar}t}|-\rangle$. (equivalently, you can show that this state fulfills the time-dependent Schrödinger equation).

e. (1 point) Calculate the probability to measure the system in the state $|\uparrow\rangle$ at a given time t.

Please turn over and use a new answer sheet

2 Symmetry of wavefunction (9 points)

We consider a Helium atom which has a doubly charged nucleus and two electrons. The two shell electrons are described by the Hamiltonian of the form

$$H = -\frac{\hbar^2}{2m}\left(\nabla_1^2 + \nabla_2^2\right) - \frac{e^2}{4\pi\epsilon_0}\left(\frac{2}{r_1} + \frac{2}{r_2} - \frac{1}{|\vec{r}_1 - \vec{r}_2|}\right) \tag{2}$$

where the subscripts '1' and '2' denote the positions of the electrons. For simplicity we neglect the electron-electron interaction and consider

$$H' = -\frac{\hbar^2}{2m}\left(\nabla_1^2 + \nabla_2^2\right) - \frac{e^2}{4\pi\epsilon_0}\left(\frac{2}{r_1} + \frac{2}{r_2}\right) \tag{3}$$

instead. H' denotes two independent electrons interacting with a nucleus of charge $2e$. If $E_1 = -13.6eV$ denotes the ground state energy of hydrogen, the ground state energy of a single electron interacting with a nucleus of charge $2e$ corresponds to $E_1' = 4E_1$ due to the stronger potential. In this question we will discuss possible electronic configurations that respect the Pauli principle. It is important to define the singlet and triplet spin states. The singlet state reads

$$|s=0; m=0\rangle = 1/\sqrt{2}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right),$$

where the first spin degree of freedom corresponds to coordinate '1' whereas the second refers to '2'. The three triplet states read

$$|s=1; m=1\rangle = |\uparrow\uparrow\rangle,$$

$$|s=1; m=0\rangle = 1/\sqrt{2}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right), \text{and}$$

$$|s=1; m=-1\rangle = |\downarrow\downarrow\rangle.$$

The total two-electron wavefunction of electrons consists of a spatial part $\psi(\vec{r}_1, \vec{r}_2)$ and a spin part $|\chi_{12}\rangle$; *i.e.*, $\Psi(\vec{r}_1, \vec{r}_2) = \psi(\vec{r}_1, \vec{r}_2) \otimes |\chi_{12}\rangle$.

a. (2 points) First, show that the singlet state is antisymmetric under exchange and that all the triplet states are symmetric.

b. (2 points) The wavefunction of a system of two electrons needs to be antisymmetric under exchange of the electrons. What are the two possibilities for the spatial part of the wavefunction $\psi(\vec{r}_1, \vec{r}_2)$ given there is a spin part?

We are now interested in the ground state of the two electron system. (Note that here $\psi_{100}(\vec{r})$ denotes the groundstate wavefunction of hydrogen with nuclear charge $+2e$)

c. (2 points) Argue that the spatial part of the wavefunction of the full system reads $\psi_1(\vec{r}_1, \vec{r}_2) = \psi_{100}(\vec{r}_1)\psi_{100}(\vec{r}_2)$. What does this mean for the spin state?

d. (2 points) What is the lowest possible energy in the case of a spin triplet? Argue whether this state is degenerate (neglecting any electron-electron and spin-orbit interactions).

e. (1 point) What is the ground state if there are two bosons in the system and how would this extend to three?

Please turn over and use a new answer sheet

3 Harmonic Oscillator (15 points)

We consider a harmonic oscillator with a perturbation. The Hamiltonian is given by

$$H = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 + H_1 \tag{4}$$

where H_1 is a perturbation given by

$$H_1 = \lambda\alpha(\hat{x} - x_0)^2 \,. \tag{5}$$

In the above expression λ is a dimensionless parameter, α has the unit kg/s^2, and x_0 is a shift. In the following exercise we will attack this problem from various angles.

We start by isolating a solvable Hamiltonian which we define as

$$H_0 = H - H_1 = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 \,. \tag{6}$$

H_0 can be solved by a series of manipulations: (1) one uses a suitable variable transformation to bring H_0 into the form

$$H_0 = \hbar\omega\left(-\frac{1}{2}\frac{d^2}{dy^2} + \frac{1}{2}y^2\right) \,. \tag{7}$$

(2) One can introduce the ladder operators $a_- = \frac{1}{\sqrt{2}}\left(y + \frac{d}{dy}\right)$ and $a_+ = \frac{1}{\sqrt{2}}\left(y - \frac{d}{dy}\right)$ which fulfil $[a_-, a_+] = 1$. The operators a_- and a_+ have the following action on the states $|n\rangle$: $a_-|n\rangle = \sqrt{n}|n-1\rangle$ ($a_-|0\rangle = 0$) and $a_+|n\rangle = \sqrt{n+1}|n+1\rangle$.

a. (2 points) Show that the Hamiltonian H_0 can be written as

$$H_0 = \hbar\omega\left(a_+a_- + \frac{1}{2}\right) \,. \tag{8}$$

b. (2 points) What are the allowable eigenvalues of H_0 ?

From now on we consider

$$H = H_0 + H_1 = \hbar\omega\left(-\frac{1}{2}\frac{d^2}{dy^2} + \frac{1}{2}y^2\right) + \lambda\left(y - y_0\right)^2 \,. \tag{9}$$

3.1 Perturbation theory

We can rewrite the perturbation $H_1 = \lambda\left(y - y_0\right)^2$ in terms of the operators a_- and a_+.

c. (2 points) Do this and derive an expression for the lowest order correction to the eigenenergies, meaning $\Delta E_n^{(1)} = \langle n|H_1|n\rangle$. $\Delta E_n^{(1)} = \langle n|H_1|n\rangle$.

3.2 Variational approach

We consider H (Eq. (9)) from a variational point of view. An ansatz for a normalized variational wave function is given by $\psi(y) = \left(\frac{2b}{\pi}\right)^{1/4} e^{-by^2}$. In the following, you can use $\langle\psi|\frac{d^2}{dy^2}|\psi\rangle = -b$ and $\langle\psi|y^2|\psi\rangle = \frac{1}{4b}$.

d. (3 points) Show that

$$\langle\psi|H|\psi\rangle = \frac{\hbar\omega}{2}\left(b + \frac{1}{4b}\right) + \lambda\left(\frac{1}{4b} + y_0^2\right). \tag{10}$$

e. (2 points) Find the optimal b_{opt} for this expression and determine the corresponding $\langle\psi|H|\psi\rangle$ (you may express this in terms of b_{opt}).

3.3 Exact solution

The Hamiltonian H of Eq. (9) can be solved exactly.

f. (3 points) Show that you can bring it into the form

$$H = \frac{\hbar\sqrt{\omega\left(\omega + \frac{2\lambda}{\hbar}\right)}}{2}\left(-\frac{d^2}{dy'} + \frac{1}{2}y'^2\right) + \frac{\lambda^2}{\frac{\hbar\omega}{2} + \lambda}y_0^2. \tag{11}$$

This leads to $E_n = \hbar\sqrt{\omega\left(\omega + \frac{2\lambda}{\hbar}\right)}\left(n + \frac{1}{2}\right) + \frac{\lambda^2}{\frac{\hbar\omega}{2}+\lambda}y_0^2$.

g. (1 point) Give a reason why the energies found in the variational approach and perturbation theory should be higher than the exact ground state energy.

End of this exam. Is every answer sheet marked with your NAME and STUDENT NUMBER?