2. exam (2. välikoe): 4 problems, 4 hours

Regarding all problems:
Consult the *collection of formulae* in the end of the problem sheet!

1. As you remember, a rotation of a state vector – formulated in terms of the standard Euler angles α, β and γ – is caused by the operator

$$\hat{D}(\alpha, \beta, \gamma) = e^{-\frac{i}{\hbar}\alpha \hat{J}_z} e^{-\frac{i}{\hbar}\beta \hat{J}_y} e^{-\frac{i}{\hbar}\gamma \hat{J}_z}$$

Let's consider a one-electron system where the orbital angular momentum $\mathbf{L} = 0$. Suppose that the system is originally in a state which is an eigenstate of the squared total angular momentum $\mathbf{J}^2$ and where the z-component of the electron's spin is up, $+\frac{\hbar}{2}$. What is the state of the system after the above rotation? Express your result in the basis $|j, m\rangle$ and in terms of coefficients functions which depend on α, β and γ. In such rotated state, what is the probability for finding the electron still with spin up?

2. (a) Using the Wigner-Eckart theorem, show that for a vector operator $\hat{\mathbf{V}}$, we have

$$\langle \xi jm|\hat{\mathbf{V}}|\xi jm'\rangle = \frac{\langle \xi jm|\hat{\mathbf{V}} \cdot \hat{\mathbf{J}}|\xi jm\rangle}{\hbar^2 j(j+1)} \langle \xi jm|\hat{\mathbf{J}}|\xi jm'\rangle$$

As an application, let's consider the Zeeman effect on the hydrogen energy levels in the following. Let the perturbation potential be

$$\hat{H}_B = \frac{\beta B}{\hbar}(\hat{L}_z + 2\hat{S}_z)$$

where B is the magnitude of the weak magnetic field which is pointing into the z direction, β is the Bohr magneton, $\hat{\mathbf{L}}$ is the orbital angular momentum and $\hat{\mathbf{S}}$ is the spin-angular momentum.

(b) We wish to apply the above result below. For this, we should show first that the operator

$$\hat{\mathbf{M}} = \hat{\mathbf{L}} + 2\hat{\mathbf{S}}$$

is a vector operator. Explain, without doing the calculation, how you would show that $\hat{\mathbf{M}}$ indeed is a vector operator.

(c) Applying the result you derived in the item (a) above, compute then the energy corrections

$$\Delta E_B^{nlj} = \langle nlsjm|\hat{H}_B|nlsjm\rangle.$$

(d) What is the energy-level splitting for the state $ns_{\frac{1}{2}}$ i.e. when $l = 0$ and $j = \frac{1}{2}$? Sketch a figure of the splitting, mark the relevant quantum numbers in the figure.

3. For a three-dimensional system, where one fermion is in a harmonic potential

$$V(\mathbf{x}) = \frac{1}{2}m\omega^2\mathbf{x}^2 = \frac{1}{2}m\omega^2(x^2 + y^2 + z^2),$$

the one-particle Hamilton operator is

$$\hat{H}^{(1)} = \frac{\hat{\mathbf{p}}^2}{2m} + V(\hat{\mathbf{x}}).$$

It is known that for such a system

$$\hat{H}^{(1)}|n_x, n_y, n_z, s_z\rangle = \epsilon_n|n_x, n_y, n_z, s_z\rangle,$$

where the eigenenergies are $\epsilon_n = \hbar\omega(n + \frac{3}{2})$, with $n = n_x + n_y + n_z$ and where $n_x, n_y, n_z = 0, 1, 2, \ldots$ and s_z is the z-component of the particle's spin.

Let us then consider N *noninteracting identical spin-$\frac{1}{2}$ fermions* moving in the potential $V(\mathbf{x})$ above. The Hamilton operator of the N-fermion system is thus

$$\hat{H} = \sum_{i=1}^{N} \hat{H}_i^{(1)} = \sum_{i=1}^{N} \left(\frac{\hat{\mathbf{p}}_i^2}{2m} + V(\hat{\mathbf{x}}_i) \right).$$

(a) Starting from the general Fock-space form of a 1-particle operator and using the 1-particle states $|n_x, n_y, n_z, s_z\rangle$ and their quantum numbers, derive the Fock-space expression of the $\hat{H}$ for this system. Express $\hat{H}$ in terms of the particle number operators and the eigenenergies ϵ_n.

(b) Form the ground state of this system for $N = 8$. Draw a diagram of the 1-particle energy levels and in the figure specify the quantum numbers of the occupied 1-particle states in such a ground state.

(c) Express the ground state $|F\rangle$ of the system explicitly as a Fock state in the occupation number representation, when $N = 8$. Express the state $|F\rangle$ also in terms of creation operators and the vacuum $|0\rangle$.

(d) Using the Fock-space form of $\hat{H}$ which you derived in the item (a) above, compute $\hat{H}|F\rangle$ explicitly for the ground state $|F\rangle$ for $N = 8$.

(e) Using the the Fock-space forms of $\hat{H}$ and the total number operator $\hat{N}$ and the anticommutation relations for the annihilation and creation operators, show that $[\hat{H}, \hat{N}] = 0$. What does this result indicate and what is the physical reason for it?

4. (a) Substituting an ansatz

$$\Psi(x) = u(p)e^{-\frac{i}{\hbar}p\cdot x}$$

into the Dirac equation

$$(i\hbar\gamma^\mu\partial_\mu - mc)\Psi(x) = 0,$$

and using the Clifford algebra for the gamma-matrices, show that the Dirac equation has both positive-energy and negative-energy solutions. Which are the allowed values of energy?

(b) Starting from the Dirac equation, and using an ansatz

$$\Psi(x) = e^{-\frac{i}{\hbar}Et}\begin{pmatrix} \psi_u(\mathbf{x}) \\ \psi_l(\mathbf{x}) \end{pmatrix},$$

show that at the non-relativistic limit the upper 2-component spinors $\psi_u(\mathbf{x})$ for the positive-energy solutions fulfill the Schrödinger equation while the lower spinors $\psi_l(\mathbf{x})$ vanish. Use the Dirac-Pauli representation here.

Collection of formulae:

Spherical coordinates and spherical harmonics:

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r}) - \frac{1}{\hbar^2 r^2}\hat{L}^2 \qquad d^3r = r^2 dr d\Omega = r^2 dr \sin\theta d\theta d\varphi \qquad \int d\Omega = 4\pi$$

$$\hat{L}^2 Y_{lm}(\theta,\varphi) = \hbar^2 l(l+1) Y_{lm}(\theta,\varphi) \qquad \hat{L}_z Y_{lm}(\theta,\varphi) = \hbar m Y_{lm}(\theta,\varphi)$$

$$\hat{L}^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial}{\partial\theta}) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right] \qquad \int d\Omega\, Y^*_{l'm'}(\theta,\varphi) Y_{lm}(\theta,\varphi) = \delta_{ll'}\delta_{mm'}$$

$$Y_{lm}(\theta,\varphi) = (-1)^{\frac{m+|m|}{2}}\sqrt{\frac{2l+1}{4\pi}}\sqrt{\frac{(l-|m|)!}{(l+|m|)!}} P_l^{|m|}(\cos\theta) e^{im\varphi} \qquad Y_{l,-m}(\theta,\varphi) = (-1)^m Y^*_{l,m}(\theta,\varphi)$$

$$P_l^k(z) = (1-z^2)^{k/2}\frac{d^k}{dz^k}P_l(z) \qquad P_l(z) = \frac{1}{2^l l!}\frac{d^l}{dz^l}(z^2-1)^l$$

$$Y_{00}(\theta,\varphi) = \frac{1}{\sqrt{4\pi}} \qquad Y_{10}(\theta,\varphi) = \sqrt{\frac{3}{4\pi}}\cos\theta \qquad Y_{1\pm1}(\theta,\varphi) = \mp\sqrt{\frac{3}{8\pi}}\sin\theta e^{\pm i\varphi}$$

$$Y_{20}(\theta,\varphi) = \sqrt{\frac{5}{16\pi}}\left(3\cos^2\theta - 1\right) \qquad Y_{2\pm1}(\theta,\varphi) = \mp\sqrt{\frac{15}{8\pi}}\cos\theta\sin\theta e^{\pm i\varphi} \qquad Y_{2\pm2}(\theta,\varphi)\sqrt{\frac{15}{32\pi}}\sin^2\theta e^{\pm 2i\varphi}$$

Transition probability, lowest order, $i \neq f$:

$$P_{fi}(t,t_0) \equiv |\langle\phi_f|\psi(t)\rangle|^2 \approx \frac{1}{\hbar^2}\left|\int_{t_0}^{t} dt_1 \langle\phi_f|\hat{V}_S(t_1)|\phi_i\rangle e^{i(E_f-E_i)t_1/\hbar}\right|^2$$

Hydrogen-like atom wave-functions:

$$\Psi_{nlm}(\mathbf{x}) = R_{nl}(r) Y_{lm}(\theta,\varphi) \qquad \kappa = \frac{Z}{na} \qquad a = \frac{4\pi\epsilon_0\hbar^2}{\mu e^2}$$

$$R_{nl}(r) = \sqrt{(2\kappa)^3\frac{(n-l-1)!}{2n(n+l)!}}(2\kappa r)^l e^{-\kappa r} L^{2l+1}_{n-l-1}(2\kappa r) \qquad L^q_p(x) = \sum_{k=0}^{p}(-1^k)\frac{(p+q)!x^k}{(p-k)!(q+k)!k!}$$

$$R_{10} = 2\left(\frac{Z}{a}\right)^{3/2} e^{-Zr/a} \qquad R_{20} = \frac{1}{\sqrt{2}}\left(\frac{Z}{a}\right)^{3/2}\left(1-\frac{Zr}{2a}\right)e^{-Zr/2a} \qquad R_{21} = \frac{1}{2\sqrt{6}}\left(\frac{Z}{a}\right)^{5/2} r e^{-Zr/2a}$$

Spherical Bessel & Neumann functions:

$$r^2\frac{d^2R(r)}{dr^2} + 2r\frac{dR(r)}{dr} + \left[(kr)^2 - l(l+1)\right]R(r) = 0 \quad \rightarrow \quad R(r) = Aj_l(kr) + Bn_l(kr)$$

$$j_l(x) = 2^l x^l\sum_{s=0}^{\infty}\frac{(-1)^s(s+l)!}{s!(2s+2l+1)!}x^{2s} \qquad n_l(x) = \frac{(-1)^{l+1}}{2^l x^{l+1}}\sum_{s=0}^{\infty}\frac{(-1)^s(s-l)!}{s!(2s-2l)!}x^{2s}$$

$$j_0(x) = \frac{\sin x}{x} \qquad j_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x} \qquad n_0(x) = -\frac{\cos x}{x} \qquad n_1(x) = -\frac{\cos x}{x^2} - \frac{\sin x}{x}$$

For integrations:

$$\int_0^\infty dx x^n e^{-ax} = \frac{n!}{a^{n+1}}, \qquad \int_{-\infty}^\infty dx e^{-ax^2} = \sqrt{\frac{\pi}{a}}, \qquad \mathrm{Res} f(z)\big|_{z=z_0} = \lim_{z\to z_0} \frac{1}{(n-1)!}\Big(\frac{d}{dz}\Big)^{n-1}[(z-z_0)^n f(z)]$$

$$\oint_C dz f(z) = 2\pi i \sum_{j=1}^n \mathrm{Res} f(z)\big|_{z=z_j}.$$

Trigonometry: $\cos 2x = \cos^2 x - \sin^2 x, \qquad \cos^2 x + \sin^2 x = 1$

Angular momentum:

$$\hat{\mathbf{J}}^2|j,m\rangle = \hbar^2 j(j+1)|j,m\rangle, \qquad \hat{J}_z|j,m\rangle = \hbar m|j,m\rangle$$

$$\hat{J}_\pm = \hat{J}_x \pm i\hat{J}_y, \qquad \hat{J}_\pm|j,m\rangle = \hbar\sqrt{(j\mp m)(j\pm m+1)}|j,m\pm 1\rangle$$

$$[\hat{J}_i, \hat{J}_j] = i\hbar\sum_{k=1}^3 \epsilon_{ijk}\hat{J}_k, \quad [\hat{\mathbf{J}}^2, \hat{J}_i] = 0$$

Power series:

$$e^x = \sum_{n=0}^\infty \frac{x^n}{n!} \qquad \cos x = \sum_{n=0}^\infty (-1)^n \frac{x^{2n}}{(2n)!} \qquad \sin x = \sum_{n=0}^\infty (-1)^n \frac{x^{2n+1}}{(2n+1)!}$$

Pauli spin matrices:

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

$$[\sigma_i, \sigma_j] = 2i\epsilon_{ijk}\sigma_k \qquad \{\sigma_i, \sigma_j\} = 2\delta_{ij}\mathbf{1}_2$$

$$(\vec{\sigma}\cdot\vec{a})(\vec{\sigma}\cdot\vec{b}) = (\vec{a}\cdot\vec{b})\mathbf{1}_2 + i(\vec{a}\times\vec{b})\cdot\vec{\sigma}$$

Wignert-Eckart theorem:

$$\langle \xi' j' m'|\hat{T}_q^{(k)}|\xi j m\rangle = \frac{1}{\sqrt{2j'+1}}\, {}_u\langle jkmq|jkj'm'\rangle_c\, \langle \xi' j'||T^{(k)}||\xi j\rangle$$

where

$$\langle \xi' j'||T^{(k)}||\xi j\rangle \equiv \frac{1}{\sqrt{2j'+1}} \sum_{m_1,m_2,q'} \langle \xi' j' m_1|\hat{T}_{q'}^{(k)}|\xi j m_2\rangle\langle jkm_2q'|jkj'm_1\rangle$$

$SU(2)$ tensor operator:

$$[\hat{J}_z, \hat{T}_q^{(k)}] = q\hat{T}_q^{(k)} \qquad [\hat{J}_\pm, \hat{T}_q^{(k)}] = \sqrt{k(k+1) - q(q\pm 1)}\,\hat{T}_{q\pm 1}^{(k)},$$

where q refers to the spherical components, which for a vector operator are

$$\hat{V}_{+1} = -\frac{1}{\sqrt{2}}(\hat{V}_x + i\hat{V}_y), \qquad \hat{V}_0 = \hat{V}_z \qquad \hat{V}_{-1} = +\frac{1}{\sqrt{2}}(\hat{V}_x - i\hat{V}_y)$$

Spherical unit vectors:

$$\hat{e}_{\pm 1} = \mp \frac{1}{\sqrt{2}}(\hat{e}_x \pm i\hat{e}_y), \qquad \hat{e}_0 = \hat{e}_z$$

Scalar products in spherical basis: $\mathbf{A} \cdot \mathbf{B} = -A_{+1}B_{-1} - A_{-1}B_{+1} + A_0 B_0$

Fermionic operators in the Fock space:

$$a_\nu |n_1 n_2 \ldots 1_\nu \ldots\rangle = (-1)^{\sum_{\mu=1}^{\nu-1} n_\mu} |n_1 n_2 \ldots 0_\nu \ldots\rangle$$

$$a_\nu^\dagger |n_1 n_2 \ldots 0_\nu \ldots\rangle = (-1)^{\sum_{\mu=1}^{\nu-1} n_\mu} |n_1 n_2 \ldots 1_\nu \ldots\rangle$$

$$\{a_\mu, a_\nu\} = 0 \qquad \{a_\mu^\dagger, a_\nu\} = \delta_{\mu\nu}$$

$$\hat{N} = \sum_\mu a_\mu^\dagger a_\mu$$

Fock space operators:

$$\hat{F} = \sum_{\mu,\nu} \langle\mu|\hat{f}|\nu\rangle a_\mu^\dagger a_\nu \qquad \hat{F} = \frac{1}{2} \sum_{\mu,\mu',\nu,\nu'} \langle\mu\mu'|\hat{g}|\nu\nu'\rangle a_\mu^\dagger a_{\mu'}^\dagger a_{\nu'} a_\nu$$

Relativistic theory:

metric tensor $g_{\mu\nu} = \mathrm{diag}(1, -1, -1, -1) = g^{\mu\nu}$

scalar products $a \cdot b = a_\mu b^\mu$

4-vectors: $x^\mu = (ct, \mathbf{x})$, $p^\mu = (E/c, \mathbf{p})$, $A^\mu = (\varphi/c, \mathbf{A})$

derivatives: $\partial_\mu = \frac{\partial}{\partial x^\mu} = (\frac{1}{c}\frac{\partial}{\partial t}, \nabla)$, and $\partial^\mu = \frac{\partial}{\partial x_\mu}$

Clifford algebra for the Dirac gamma-matrices: $\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu}\mathbf{1}_4$

Dirac-Pauli representation:

$$\gamma^0 = \begin{pmatrix} \mathbf{1}_2 & 0 \\ 0 & -\mathbf{1}_2 \end{pmatrix} \qquad \gamma^i = \begin{pmatrix} 0 & \sigma^i \\ -\sigma^i & 0 \end{pmatrix}$$

Some more Taylor series expansions:

$$\sqrt{1+x} = 1 + \frac{1}{2}x - \frac{1}{8}x^2 + \ldots \qquad \ln(1+x) = x - \frac{1}{2}x^2 + \frac{1}{3}x^3 + \ldots$$