UNIVERSITY OF CAMBRIDGE

NATURAL SCIENCES TRIPOS Part II

Wednesday 27 April 2022, 10.30 to 12.30

THEORETICAL PHYSICS 2

*Answer **all four** questions.*

The approximate number of marks allotted to each part of a question is indicated in the right margin where appropriate.

The paper contains **five** *sides, including this one, and is accompanied by a booklet giving values of constants and containing mathematical formulae which you may quote without proof. (The booklet is available for separate download.)*

V7.1

1 Consider the following Hamiltonian for a spin-1 degree of freedom in a magnetic field:

$$H = \mathbf{B} \cdot \mathbf{S},$$

where $\mathbf{S} = (S_x, S_y, S_z)$ and $\mathbf{B} = B_0(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$.

(a) Write the explicit Hamiltonian in terms of the *spin-1* matrices $S_{x,y,z}$ in the $|m_z\rangle$-basis, where $m_z = -1, 0, 1$ for $s = 1$.
[*Hint: Recall that for spin-s, the raising and lowering operators act as* $S_\pm|s, m_s\rangle = \sqrt{s(s+1) - m_s(m_s \pm 1)}|s, m_s\rangle$. *Note that* $|m_z\rangle \equiv |s = 1, m_s\rangle$.] [2]

(b) Use a 'rotated frame' transformation $U(\theta, \phi) = e^{i\phi S_z} e^{i\theta S_y} \equiv U(\phi)U(\theta)$ to show that

$$H = U(\theta, \phi) H_z (U(\theta, \phi))^\dagger,$$

in terms of $H_z = B_0 S_z$.
[*Hint: Recall that* $e^X Y e^{-X} = Y + [X, Y] + \frac{1}{2!}[X, [X, Y]] + \frac{1}{3!}[X, [X, [X, Y]]] + ...$] [8]

The eigenstates of H are thus given by $|B, m_z\rangle = U(\theta, \phi)|m_z\rangle$.

(c) Show that the explicit form of the eigenstate with highest eigenvalue, $|B, +1\rangle = U(\theta, \phi)|m_z = 1\rangle$, is given by [7]

$$|B, +1\rangle = \begin{pmatrix} e^{-i\phi}\cos^2(\theta/2) \\ \sqrt{2}\sin(\theta/2)\cos(\theta/2) \\ e^{i\phi}\sin^2(\theta/2) \end{pmatrix}.$$

(d) Show that the Berry potential $\mathbf{A}_+ = -i\langle B, +1|\nabla|B, +1\rangle$ is [5]

$$-\frac{1}{B_0}\cot(\theta)\,\hat{\phi}.$$

(e) Writing $\mathbf{B} = B_0\hat{\mathbf{n}}$, show that the Berry curvature is given by $\frac{\hat{\mathbf{n}}}{B_0^2}$. What does this expression physically mean? Predict a general relation for a spin-s degree of freedom in a magnetic field with the same Hamiltonian as above. [3]

Solution 1. (a) *[Unseen but very similar to derivation addressed in Lecture.]*

Given the eigenstates $|m_z\rangle$ of S_z, $S_z|m_z\rangle = m_z|m_z\rangle$, $S_\pm$ act in the usual manner, increasing or decreasing m_z and annihilating the top/bottom state to zero, respectively. Hence,

$$S_+ = \sqrt{2}\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} \tag{1}$$

and

$$S_- = \sqrt{2}\begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}. \tag{2}$$

Consequently,

$$S_x = \frac{1}{2}(S_+ + S_-) = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \tag{3}$$

and

$$S_y = -\frac{i}{2}(S_+ - S_-) = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}. \tag{4}$$

The Hamiltonian is thus given as

$$H = \frac{B_0}{\sqrt{2}}\Bigg[\sin(\theta)\cos(\phi)\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \tag{5}$$

$$+ \sin(\theta)\sin(\phi)\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} + \cos(\theta)\begin{pmatrix} \sqrt{2} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -\sqrt{2} \end{pmatrix}\Bigg] \tag{6}$$

(b) We need to evalaute $U(\phi)U(\theta)S_zU(\theta)^\dagger U(\phi)^\dagger$. We proceed via two steps.

Step 1: $U(\phi)S_zU(\theta)^\dagger U(\phi)$. We evaluate $e^{-i\theta S_y}S_ze^{i\theta S_y}$. We use

$$e^ABe^{-A} = B + [A,B] + 1/(2!)[A,[A,B] + 1/(3!)[A,[A,[A,B] + ..., \tag{7}$$

where $B = S_z$ and $A = -i\theta S_y$. We then obtain

$$\begin{aligned} S_z & +(-i\theta)(iS_x) + 1/(2!)(-i\theta)^2[S_y, iS_z] + 1/(3!)(-i\theta)^3[S_y,[S_y,[S_y,S_z] + ... \quad (8) \\ = & \; S_z + (-i\theta)(iS_x) + 1/(2!)(-i\theta)^2[S_y, iS_x] + 1/(3!)(-i\theta)^3[S_y,[S_y,[S_y,S_z] + ... \\ = & \; S_z + \theta S_x - 1/(2!)(\theta)^2S_z + 1/(3!)(-i\theta)^3[S_y,S_z] + ... \\ = & \; S_z + \theta S_x - 1/(2!)(\theta)^2S_z - /(3!)(\theta)^3S_x + ... \\ = & \; S_z\cos(\theta) + S_x\sin(\theta). \quad (9) \end{aligned}$$

Step 2: We do the same for $e^{-i\phi S_z}(S_z\cos(\theta)+S_x\sin(\theta))e^{i\phi S_z}$. Note that the first term commutes with S_z and thus $U(\phi)$ can be cancelled with $(U(\phi))^\dagger$. For $e^{-i\phi S_z}(S_x\sin(\theta))e^{i\phi S_z}$ we note that this is the same problem as above with the same commutation relations, but with S_z replaced by S_x, S_y by S_z and S_x by S_y. Hence this term gives

$$\sin(\theta)\cos(\phi)S_x+\sin(\theta)\cos(\phi)S_y. \tag{10}$$

In total we thus get

$$U(\phi)U(\theta)S_zU(\theta)^\dagger U(\phi)^\dagger=\sin(\theta)\cos(\phi)S_x+\sin(\theta)\cos(\phi)S_y+\cos(\theta)S_z, \tag{11}$$

and, upon filling in the prefactor, one finds the desired result.

(c) *[Unseen.]* We need to evaluate $U(\theta)$ and $U(\phi)$. Note that S_z is diagonal and hence

$$U(\phi)=\begin{pmatrix} e^{i\phi} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & e^{-i\phi}\end{pmatrix}. \tag{12}$$

To evaluate $U(\theta)$ we exponentiate. We note that $S_y^3=S_y$, hence we get

$$\begin{aligned} U(\theta) &= 1+(-i\theta)S_y+(-i\theta)^2/2S_y^2+(-i\theta)^3/(3!)S_y^3+(-i\theta)^4/(4!)S_y^4+... &(13)\\ &= 1+(-i\theta)S_y+(-i\theta)^2/2S_y^2+(-i\theta)^3/(3!)S_y+(-i\theta)^4/(4!)S_y^2+... \\ &= \sinh(i\theta)S_y+\cos(\theta)S_y^2+(1-S_y^2). &(14)\end{aligned}$$

In matrix form this gives

$$U(\theta)=\begin{pmatrix} 1/2+1/2\cos(\theta) & -1/\sqrt{2}\sin(\theta) & 1/2-1/2\cos(\theta) \\ 1/\sqrt{2}\sin(\theta) & \cos(\theta) & -1/\sqrt{2}\sin(\theta) \\ 1/2-1/2\cos(\theta) & 1/\sqrt{2}\sin(\theta) & 1/2+1/2\cos(\theta)\end{pmatrix}. \tag{15}$$

Using that $|m_z=+1\rangle=(1,0,0)^T$ and the doubling formulae

$$1/2+1/2\cos(\theta)=\cos^2(\theta/2) \tag{16}$$
$$2\sin(\theta)\cos(\theta)=\sin(2\theta) \tag{17}$$
$$1/2-1/2\cos(\theta)=\sin^2(\theta/2) \tag{18}$$

we find that, upon multiplying, $|B,+1\rangle=U(\theta,\phi)|m_z=1\rangle$ is given by

$$|B,+1\rangle=\begin{pmatrix} e^{-i\phi}\cos^2(\theta/2) \\ \sqrt{2}\sin(\theta/2)\cos(\theta/2) \\ e^{i\phi}\sin^2(\theta/2)\end{pmatrix}. \tag{19}$$

(d) *[Unseen.]*

We first calculate $\nabla|B,+1\rangle$. We find

$$\begin{aligned}\nabla|B,+1\rangle &= \frac{1}{B_0}\partial_\theta|B,+1\rangle\hat{\theta} + \frac{1}{B_0\sin(\theta)}\partial_\theta|B,+1\rangle\hat{\phi} \quad (20)\\ &= \frac{1}{B_0}\begin{pmatrix} e^{-i\phi}\cos(\theta/2)sin(\theta/2) \\ \sqrt{2}\cos^2(\theta/2)-\sin^2(\theta/2)]/2 \\ e^{i\phi}\sin(\theta/2)\cos(\theta/2)\end{pmatrix}\hat{\theta} + \frac{1}{B_0\sin(\theta)}\begin{pmatrix}-ie^{-i\phi}\cos^2(\theta/2) \\ 0 \\ ie^{i\phi}\sin^2(\theta/2)\end{pmatrix}\hat{\phi}.\end{aligned}$$

As a next step we evaluate $\langle B,+1|\nabla|B,+1\rangle$ and find

$$\begin{aligned}\langle B,+1|\nabla|B,+1\rangle &= \frac{1}{B_0}[-\cos^2(\theta/2)[\cos(\theta/2)\sin(\theta/2)] \\ &+ \sin(\theta/2)\cos(\theta/2)[\cos^2(\theta/2)-\sin^2(\theta/2)]+\sin^3(\theta/2)\cos(\theta/2)]\hat{\theta} \\ &+ [-i\cos^3(\theta/2)+i\sin^3(\theta/2)]\hat{\phi}/(r\sin(\theta)) \\ &= \frac{i}{B_0\sin(\theta)}[\sin^4(\theta/2)-cos^4(\theta/2)]\hat{\phi} \\ &= \frac{i}{B_0\sin(\theta)}[\sin^2(\theta/2)+cos^2(\theta/2)][\sin^2(\theta/2)-cos^2(\theta/2)]\hat{\phi} \\ &= \frac{i}{B_0\sin(\theta)}[\sin^2(\theta/2)-cos^2(\theta/2)]\hat{\phi} \\ &= \frac{-i}{B_0\sin(\theta)}[\cos(\theta)]\hat{\phi} \\ &= -\frac{i}{B_0}\cot(\theta)\hat{\phi}. \quad (21)\end{aligned}$$

Hence, $\mathbf{A}_+ = -\frac{1}{B_0}\cot(\theta)\hat{\phi}$.

(e) *[Same as in lecture]*

To evaluate the Berry curvature we simple take the divergence. Using $\mathbf{B} = B_0\hat{\mathbf{n}}$,

$$\begin{aligned}\nabla\times\mathbf{A}_+ &= \frac{1}{B_0\sin(\theta)}\partial_\theta[\sin(\theta)(-1/B_0\cot(\theta))]\hat{\mathbf{n}} \quad (22)\\ &= \frac{\hat{\mathbf{n}}}{B_0^2}. \quad (23)\end{aligned}$$

Integrating gives twice the result in terms of solid angle as compared to spin-1/2. In other words, we now have a monopole with twice the value. Generally the relation to spin is given by a monopole charge of $\sim \frac{s}{2B_0^2}$.

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2 Consider a one-dimensional potential of strength $V_0 > 0$ of the form,

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

A solution of the scattering problem with energy $E = \frac{\hbar k^2}{2m}$ is a solution of the integral equation

$$\Psi_k(x) = e^{ikx} + \int_{-\infty}^{\infty} \mathrm{d}x' G_k^+(x,x')V(x')\Psi_k(x').$$

(a) Show that the retarded Green's function for this system is $G_k^+(x,x') = -\frac{im}{\hbar^2 k} e^{ik|x-x'|}$. $G_k^+(x,x')$ can also be written as the position matrix elements of an operator $\hat{O}$. Give an expression of $\hat{O}$. [11]

(b) By writing the wave function far away from the scatterer ($|x| \to \infty$) as

$$\Psi_k(x) \approx e^{ikx} + e^{ik|x|} f(k,k'),$$

for $k' = k\,\mathrm{sgn}(x)$, find an expression for the scattering amplitude $f(k,k')$ in terms of V_0 and a. [5]

(c) For waves incident from the left ($x \to -\infty$), find the incident, reflected and transmitted waves and their respective probability currents j_i, j_r and j_t in terms of $f(k,k')$. Determine the transmission, $T = j_t/j_i$, and reflection, $R = j_r/j_i$, coefficients. Show that the scattering amplitude must satisfy

$$\mathrm{Re}\{f(k,k)\} = -\frac{1}{2}\{|f(k,k)|^2 + |f(k,-k)|^2\}$$

for the probability to be conserved. [5]

(d) As a limiting case, consider a delta function potential $V(x) = g\delta(x)$, of strength g, and determine the scattering amplitude $f(k)$. (Notice that in this case $f(k)$ depends on only one reciprocal wave vector.) [4]

Solution 2. (a)*[Familiar problem studied in lecture.]* Lippmann-Schwinger Equation inserted into the Schrödinger equation,

$$\begin{aligned}-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial_x^2}\Psi_k(x)+V(x)\Psi_k(x) &= E_k\Psi_k(x)\\ \left[E_k+\frac{\hbar^2}{2m}\frac{\partial^2}{\partial_x^2}\right]\Psi_k(x) &= V(x)\Psi_k(x)\end{aligned}$$

means that

$$\left[E_k+\frac{\hbar^2}{2m}\frac{\partial^2}{\partial_x^2}\right]G_k^+(x,x')=\delta(x-x').$$

Using Fourier transform $G_k^+=\frac{1}{2\pi}\int \mathrm{d}qe^{iq(x-x')}\tilde{G}_k^+(q)$, we obtain

$$\begin{aligned}\frac{1}{2\pi}\int dqe^{iq(x-x')}\left[E_k+\frac{\hbar^2q^2}{2m}\right]\tilde{G}_k^+(q) &= \frac{1}{2\pi}\int dqe^{iq(x-x')},\\ \tilde{G}_k^+(q) &= \left[\frac{\hbar^2k^2}{2m}+\frac{\hbar^2q^2}{2m}+i\epsilon\right]^{-1}\end{aligned}$$

where $+i\epsilon$ is added for convergence and the contour is closed correspondingly to the boundary conditions, i.e. from top around the left pole at $-k$ and from below around the right pole at $+k$. Inserting $\tilde{G}_k^+(q)$ back for,

$$\begin{aligned}G_k^+(x,x') &= \frac{1}{2\pi}\int_{\infty}^{\infty}dq\frac{e^{iq(x-x')}}{\frac{\hbar^2k^2}{2m}+\frac{\hbar^2q^2}{2m}+i\epsilon} \qquad (24)\\ &= \frac{2im}{\hbar^2}\left[\Theta(x-x')\frac{e^{ik(x-x')}}{2k}-\Theta(x'-x)\frac{e^{ik(x'-x)}}{-2k}\right]=-\frac{im}{\hbar^2k}e^{ik|x-x'|}.\end{aligned}$$

By looking at this expression, one can see that the position matrix elements of the operator $\hat{O}=\frac{1}{E_k-H_0+i\epsilon}$ is the Green's function (for $E_k=\frac{\hbar^2k^2}{2m}$):

$$\begin{aligned}\langle x|\frac{1}{E_k-H_0+i\epsilon}|x'\rangle &= \int dq\langle x|q\rangle\langle q|\frac{1}{E_k-H_0+i\epsilon}|x'\rangle\\ &= \int\frac{dq}{2\pi}e^{iq(x-x')}\frac{1}{\frac{\hbar^2k^2}{2m}+\frac{\hbar^2q^2}{2m}+i\epsilon}.\end{aligned}$$

This equals the Fourier transform of the Green's function calculated in the first part above.

(b) *[Unseen but familiar from lecture.]*

To approximate the retarded Green's function for $|x|\to\infty$, we use

$$|x-x'|=\sqrt{(x-x')^2}\approx\sqrt{x^2-2xx'}\approx|x|-x'\frac{|x|}{x},$$

which gives

$$G_k^+(x,x')\approx-\frac{im}{\hbar^2k}e^{ik|x|-ik'x'},$$

with $k' = k|x|/x$. Lippmann-Schwinger equation takes the form

$$\Psi_k(x) \approx e^{ikx} - \frac{im}{\hbar^2 k} e^{ik|x|} \int dx' e^{-ik'x'} V(x') \Psi_k(x'),$$

with the scattering amplitude

$$f(k,k') = -\frac{im}{\hbar^2 k} \int dx' e^{-ik'x'} V(x') \Psi_k(x').$$

(c) *[Unseen but builds on the calculations in the handout.]*

Asymptotic wave functions take the form $e^{ikx} + f(k,-k)e^{-ikx}$ in the far left $x \ll 0$ and $e^{ikx} + f(k,k)e^{ikx}$ in the far right $x \gg 0$. This means (up to normalization constants),

- •The incident wave $\Psi_k^i(x) = e^{ikx}$, and the incident current $j_i(x) = \frac{\hbar k}{m}$,
- •The reflected wave $\Psi_k^r(x) = f(k,-k)e^{-ikx}$, and the reflected current $j_r(x) = -\frac{\hbar k}{m}|f(k,-k)|^2$,
- •The transmitted wave $\Psi_k^t(x) = (1 + f(k,k))e^{ikx}$, and the transmitted current $j_t(x) = \frac{\hbar k}{m}|1 + f(k,k)|^2$,

where the current is calculated by using $j(x) = -\frac{i\hbar}{2m}[\Psi^* \partial_x \Psi - \Psi \partial_x \Psi^*]$.

This gives the transmission and reflection coefficients as,

$$T = |1 + f(k,k)|^2, \quad R = |f(k,-k)|^2.$$

Since the probability is conserved, $T + R = 1$,

$$\begin{aligned} |1 + f(k,k)|^2 + |f(k,-k)|^2 &= 1 \\ \mathrm{Re}\{f(k,k)\} &= -\frac{1}{2}\{|f(k,k)|^2 + |f(k,-k)|^2\}. \end{aligned}$$

(d)

Scattering amplitude for the delta function potential is

$$f(k) = -\frac{im}{\hbar^2 k} \int dx' e^{-ik'x'} g\delta(x') \Psi_k(x') = -\frac{img}{\hbar^2 k} \Psi_k(0).$$

$\Psi_k(0)$ can be calculated from the Lippmann-Schwinger equation as $\Psi_k(0) = \frac{i\hbar^2 k/m}{i\hbar^2 k/m - g}$, which gives

$$f(k) = \frac{g}{i\hbar^2 k/m - g}.$$

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3 The Helium atom has Hamiltonian $H = H_0 + H_{12}$, where

$$H_0 = \frac{1}{2m}\left[\mathbf{p}_1^2 + \mathbf{p}_2^2\right] - 2e^2\left[\frac{1}{|\mathbf{r}_1|} + \frac{1}{|\mathbf{r}_2|}\right], \quad H_{12} = \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|}.$$

(a) We first address the spin part. Show that the two spins can form a triplet χ_{1,m_s} (with $m_s = -1, 0, 1$) or singlet $\chi_{0,0}$ ($m_s = 0$) wave function. Express them in the S_z-eigenstate basis, $|\uparrow\rangle$ and $|\downarrow\rangle$. What are their symmetry properties? [3]

(b) What is the symmetry property of fermionic states? Give the form of the ground state if H_{12} is ignored. You may use, without derivation, the fact that the Hydrogen problem has eigenfunctions $\psi_{nlm}(\mathbf{r})$ with eigenenergies $E_{nlm} \propto -e^4/(2\hbar n^2)$, for principal quantum number n, azimuthal quantum number $l = 0, 1, ..., n-1$ and magnetic quantum number $m = -l, ..., +l$.
[*Hint: Consider decomposing the wave function into a spatial part and spin part. The latter can be left implicit.*] [5]

(c) Determine the set of degenerate eigenstates of the next energy level using the same analysis as in (b). [6]

(d) Consider now the repulsion term H_{12} as a perturbation and give an expression for the correction to the ground state energy. [6]

[*Hint: Use here that,*

- *The wave function of the Hydrogen 1s state $\psi_{1,0,0}(r)$ reads $1/\sqrt{a_0^3\pi}e^{-r/a_0}$. Note that a_0 needs to be replaced with $a_0/2$ to account for the atomic nucleus in Helium.*
- $\int d\phi_1 \int d(\cos\theta_1) \int d\phi_2 \int d(\cos\theta_2) \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} = 8\pi^2 \int d(\cos\theta) \frac{1}{\sqrt{r_1^2 + r_2^2 - 2r_1 r_2\cos\theta}}$
$= \frac{8\pi^2}{r_1 r_2}(r_1 + r_2 + |r_1 - r_2|)$.
- $\int_0^\infty dx\, x\, e^{-4x} \int_0^\infty dy\, y\, e^{-4y}(x + y + |x - y|) = \frac{5}{2048}$.

]

(e) The "classical" expression for density-density fluctuations,

$$H_{int} = \frac{1}{2}\int d\mathbf{r}\, d\mathbf{r}'\, \rho(\mathbf{r}) U(\mathbf{r} - \mathbf{r}') \rho(\mathbf{r}'),$$

needs to be modified when ρ is expressed in second quantized form since the ordering for indistinguishable particles matters. Give the correct expression of the expectation value for both fermionic and bosonic product states in terms of the density operator $\rho(\mathbf{r})$ and the single particle density matrix $g(\mathbf{r}, \mathbf{r}')$, and comment on the result. [5]

Solution 3. (a) *[Seen but builds on discussion of the Lectures.]* We can start from the maximal state $|S=1, m_z=1\rangle$ and use $S_- = S_-^1 + S_-^2$. This gives the triplet

$$\begin{aligned} |11\rangle &= |\uparrow_1\rangle|\uparrow_2\rangle \\ |10\rangle &= 1/\sqrt{2}[|\uparrow_1\rangle|\downarrow_2\rangle + |\downarrow_1\rangle|\uparrow_2\rangle] \\ |1-1\rangle &= |\downarrow_1\rangle|\downarrow_2\rangle. \end{aligned}$$

The state $|S=0, m_z=0\rangle$ is the one that is orthogonal to $|S=1, m_z=0\rangle$ and reads

$$\chi_{0,0} = |00\rangle = 1/\sqrt{2}[|\uparrow_1\rangle|\downarrow_2\rangle - |\downarrow_1\rangle|\uparrow_2\rangle] \tag{25}$$

the triplets are symmetric, the singlet is anti-symmetric.

(b) *[Basic manipulation based on lecture notes.]*

The fermionic nature implies that the wave function is anti-symmetric. We can use the eigenfucntions of the Hydrogen atom as product basis. For the spin we can have a singlet or triplet, see part (a). Now as the energy depends on n, we can minimize by taking for the spatial part two radial functions with $n=1$ and s quantum number, that is $\psi(\mathbf{r}_1, \mathbf{r}_2) = \psi_{1,0,0}(r_1)\psi_{1,0,0}(r_2)$. Hence, to make it anti-symmetric the spin part has to be the singlet. We thus obtain

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = \psi_{1,0,0}(r_1)\psi_{1,0,0}(r_2)\chi_{00} \tag{26}$$

(c) *[Basic manipulation based on lecture notes.]*

We do the same analysis as (b), but now combine a $\psi_{(1,0,0)}$ with a $2s$ or $2p$ state. Hence, the spatial part needs be of the form

$$\psi_{12}^{\pm} = \frac{1}{\sqrt{2}}[\psi_{1,0,0}(\mathbf{r}_1)\psi_{2,l,m_l}(\mathbf{r}_2) \pm \psi_{2,l,m_l}(\mathbf{r}_1)\psi_{1,0,0}(\mathbf{r}_2)]. \tag{27}$$

To make the wave function anti-symmetric, the symmetric spatial part is combined with the singlet, whereas the anti-symmetric spatial part is combined with the triplet

$$\Psi_{12;0,0}^{+}(\mathbf{r}_1, \mathbf{r}_2) = \psi_{12}^{+}(\mathbf{r}_1, \mathbf{r}_2)\chi_{0,0} \tag{28}$$

$$\Psi_{12;1,m_s}^{-}(\mathbf{r}_1, \mathbf{r}_2) = \psi_{12}^{-}(\mathbf{r}_1, \mathbf{r}_2)\chi_{1,m_s}. \tag{29}$$

(d) *[Basic algebra seen in lecture]*

Taking $\psi_{1,0,0}$ and substituting with $a_0 \to a_0/2$, we get

$$\begin{aligned} \Delta_{12} &= e^2 \int d^3r_1 \int d^3r_2 \psi_{1,0,0}(r_1) \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \psi_{1,0,0}(r_2) \\ &= (64e^2)/(\pi^2 a_0^6) \int r_1^2 e^{-4r_1/a_0} dr_1 \int r_2^2 e^{-4r_2/a_0} y_{12} dr_2, \end{aligned} \tag{30}$$

where $y_{12} = \int d\theta_1 d\phi_1 \int d\theta_2 d\phi_2 \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}$. Using the formulae provided we get directly $\Delta_{12} = 5e^2/(4a_0)$.

(e) *[Familiar problem]*

As discussed in the course, the operator needs normal ordering to remove spurious self correlations. The correct form is

$$H_{int} = 1/2 \int \mathrm{d}\mathbf{r}\mathrm{d}\mathbf{r}' : \rho(\mathbf{r}) U(\mathbf{r}-\mathbf{r}') \rho(\mathbf{r}') : \tag{31}$$

For product states, having terms as $< \hat{a}^\dagger_\alpha \hat{a}_\beta \hat{a}^\dagger_\gamma \hat{a}_\delta >$, we can use Wick's theorem. We get, using the completeness relation of the wave function parts,

$$\begin{aligned} < \rho(\mathbf{r})\rho(\mathbf{r}') > &= \sum_{\alpha,\gamma} \varphi^*_\alpha(\mathbf{r})\varphi_\alpha(\mathbf{r})\varphi^*_\gamma(\mathbf{r}')\varphi_\gamma(\mathbf{r}') N_\alpha N_\gamma + \\ &+ \sum_{\alpha,\gamma} \varphi^*_\alpha(\mathbf{r})\varphi_\gamma(\mathbf{r})\varphi^*_\gamma(\mathbf{r}')\varphi_\alpha(\mathbf{r}') N_\alpha (1 \pm N_\gamma) \\ &= < \rho > \delta(\mathbf{r}-\mathbf{r}') + < \rho(\mathbf{r}) >< \rho(\mathbf{r}') > \pm g(\mathbf{r},\mathbf{r}') g(\mathbf{r}',\mathbf{r}). \end{aligned} \tag{32}$$

Upon normal ordering the first term drops and

$$\begin{aligned} : H_{int} : &= 1/2 \int \mathrm{d}\mathbf{r}\mathrm{d}\mathbf{r}' < \rho(\mathbf{r}) > U(\mathbf{r}-\mathbf{r}') < \rho(\mathbf{r}') > \\ &\pm 1/2 \int \mathrm{d}\mathbf{r}\mathrm{d}\mathbf{r}' g(\mathbf{r},\mathbf{r}') U(\mathbf{r}-\mathbf{r}') g(\mathbf{r}',\mathbf{r}). \end{aligned} \tag{33}$$

The first terms is the Hartree term the second term the Fock term. For bosons they increase due to Bunching, for fermions the Fock term reduces the overall result and relates to Pauli principle.

4 Consider two spin-1/2 particles in the state

$$|\Phi\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_1|\downarrow\rangle_2 + |\downarrow\rangle_1|\uparrow\rangle_2\right).$$

(a) Imagine that we perform a measurement of $S_{z,1}$ to determine the z-component of the spin of the first particle. Comment on whether the result of a simultaneous measurement of $S_{z,2}$ can always be predicted from the first measurement. [4]

(b) Determine the two-spin density matrix ρ corresponding to the state $|\Phi\rangle$ and compute the reduced density matrix for the first particle $\rho_{1,\mathrm{red}} = \mathrm{tr}_2[\rho]$ by tracing out the second spin. Then calculate the degree of entanglement, $S_{\mathrm{ent}} = -\mathrm{tr}[\rho_{1,\mathrm{red}} \log \rho_{1,\mathrm{red}}]$, between the two particles and comment on the purity of ρ and $\rho_{1,\mathrm{red}}$. [6]

(c) Now, consider the state

$$|\Psi\rangle = \frac{1}{2}\left(|\uparrow\rangle_1|\uparrow\rangle_2 + |\downarrow\rangle_1|\uparrow\rangle_2 + |\uparrow\rangle_1|\downarrow\rangle_2 + |\downarrow\rangle_1|\downarrow\rangle_2\right),$$

and determine the reduced density matrix $\rho_{1,\mathrm{red}}$ in this case. Find the degree of entanglement. How does your result compare with the one obtained in (b)? [5]

Now, consider a single spin-1/2 particle in the state $|S_z,+\rangle = |\uparrow\rangle$.

(d) Imagine that the particle is going through a Stern-Gerlach device oriented in the $x-z$ plane, $\hat{n} = -\sin\theta\hat{e}_x + \cos\theta\hat{e}_z$. Determine the probability of measuring the outgoing particle in the $|S_n,+\rangle$ state (the state with eigenvalue $+\frac{1}{2}$). [5]

(e) Consider a variable Stern-Gerlach device which can have one of three different orientations with equal probability,

$$\begin{aligned}
\hat{n}_1 &= -\sin\theta\hat{e}_x + \cos\theta\hat{e}_z,\\
\hat{n}_2 &= -\sin(\theta - \frac{2\pi}{3})\hat{e}_x + \cos(\theta - \frac{2\pi}{3})\hat{e}_z,\\
\hat{n}_3 &= -\sin(\theta + \frac{2\pi}{3})\hat{e}_x + \cos(\theta + \frac{2\pi}{3})\hat{e}_z.
\end{aligned}$$

For an incoming particle in state $|S_z,+\rangle$, determine the probability of measuring the eigenvalue $+\frac{1}{2}$ after the particle has traversed the device. [5]

Solution 4. (a) *[Seen in Lecture.]*

The measurement $S_{z,1}$ on state $|\Phi\rangle$ can give $\pm 1/2$ ($\hbar = 1$) with probability $1/2$ each. Measuring $|S_z+\rangle_1$ means the second particle must be in $|\downarrow\rangle_2$ state, while if we measure $-1/2$ for the first particle, the second must be in $|\uparrow\rangle_2$ state. The first measurement on the first spin fixes the second spin since the two particles are entangled.

(b) *[Familiar from lecture notes.]*

The two-spin density matrix calculated via $\rho = |\Phi\rangle\langle\Phi|$ is,

$$\rho = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1/2 & 1/2 & 0 \\ 0 & 1/2 & 1/2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

in the basis of $|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle$.

Tracing out the second spin gives,

$$\rho_{1,\text{red}} = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$$

which means the degree of entanglement is

$$S_{\text{ent}} = -\text{tr}[\rho_{1,\text{red}} \log \rho_{1,\text{red}}] = -2\frac{1}{2}\log\frac{1}{2} = \log 2.$$

ρ is a pure state since $\rho^2 = \rho$ and $\rho_{1,\text{red}}$ corresponds to a mixed state as expected since the particles are entangled.

(c) *[Unseen but familiar]*

$|\Psi\rangle$ can be written as a product state as

$$|\Psi\rangle = \left[\frac{1}{\sqrt{2}}(|\uparrow\rangle_1 + |\downarrow\rangle_1)\right] \otimes \left[\frac{1}{\sqrt{2}}(|\uparrow\rangle_2 + |\downarrow\rangle_2)\right],$$

hence the reduced density matrix

$$\rho_{1,\text{red}} = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

is pure and the degree of entanglement vanishes

$$S_{\text{ent}} = -\text{tr}[\rho_{1,\text{red}} \log \rho_{1,\text{red}}] = -\sum_i \lambda_i \log \lambda_i = 0,$$

where $\lambda_i = 0, 1$ are the eigenvalues of $\rho_{1,\text{red}}$.

While state $|\Phi\rangle$ corresponds to an entangled state, $|\Psi\rangle$ is a product state which does not carry entanglement and hence the reduced density matrices for for the two individual particles correspond to pure states.

(d) *[Unseen, but builds on examples in the lecture notes]*

We find the eigenvalues for $\boldsymbol{S} \cdot \hat{n}|S_n, \pm\rangle = \pm\frac{1}{2}|S_n, \pm\rangle$ represented in matrix form

$$\begin{pmatrix} \cos\theta & -\sin\theta \\ -\sin\theta & -\cos\theta \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \pm \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

as

$$|S_n, +\rangle = \begin{pmatrix} \cos(\theta/2) \\ -\sin(\theta/2) \end{pmatrix}, \quad |S_n, -\rangle = \begin{pmatrix} \sin(\theta/2) \\ \cos(\theta/2) \end{pmatrix}.$$

The probability of measuring $+1/2$ for the outgoing particle is then

$$|\langle S_z, +\rangle|S_n, +\rangle|^2 = \cos^2(\theta/2).$$

(e) *[Unseen, but builds on examples in the lecture notes]*

From the result in part (d) one can see that the probability of measuring spin eigenvalue $+1/2$ for each of the Stern-Gerlach orientations $\hat{n}_i$ is given by $\cos^2(\frac{\theta}{2} + \phi_i)$ with $\phi_i = \{0, -2\pi/3, 2\pi/3\}$. The orientation $\hat{n}_i$ is however decided with a classical probability with equal weight. We then sum all the probabilities

$$P = \frac{1}{3}\left\{ \cos^2(\frac{\theta}{2}) + \cos^2(\frac{\theta}{2} - \frac{\pi}{2}) + \cos^2(\frac{\theta}{2} + \frac{\pi}{2}) \right\} = \frac{1}{2}.$$
