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Solution to Exam in: FYS3110 - Quantum mechanics.

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Max score: 56 points

Problem 1

1a)(6 points) A hermitian operator is an operator that is equal to its hermitian conjugate: $\hat{K} = \hat{K}^\dagger$.

Properties of hermitian operators (see Griffiths, chapter 3):

- Real eigenvalues. Eigenvalues correspond to measurement values, they should be real.
- Eigenstates with different eigenvalues are orthogonal. Eigenstates are states for which the measurement value is the corresponding eigenvalue with 100% certainty. Physical states that for sure give different measurement values must be orthogonal.
- Eigenstates span the Hilbert space¹. It must be possible to assign probabilities for getting a particular measurement value for *any* state. This means that it must be possible to write any state as a superposition of eigenstates. This is the spanning or completeness property.

Grading: 1.5 points for giving the correct definition. 1.5 for mentioning real eigenvalues, 1.5 for mentioning orthogonality of eigenfunctions, and 1.5 for mentioning the spanning property.

¹ The last property is not automatic for hermitian operators in an ∞ -dimensional Hilbert space.

1b)(6 points) The hermitian conjugate of $\hat{M} = ix \frac{d}{dx}$

$$\begin{aligned}
 \langle \psi | \hat{M}^\dagger | \psi \rangle &= \langle \psi | \hat{M} | \psi \rangle^* = \left[\int_{-\infty}^{\infty} dx \psi^*(x) ix \frac{d}{dx} \psi(x) \right]^* = -i \int_{-\infty}^{\infty} dx \psi(x) x \frac{d}{dx} \psi^*(x) \\
 &= -i \int_{-\infty}^{\infty} dx \left[\frac{d}{dx} (\psi(x) x \psi^*(x)) - \frac{d}{dx} (\psi(x) x) \psi^*(x) \right] \\
 &= -i [\psi(x) x \psi^*(x)]_{-\infty}^{\infty} + i \int_{-\infty}^{\infty} dx \frac{d}{dx} (\psi(x) x) \psi^*(x) \\
 &= 0 + i \int_{-\infty}^{\infty} dx \psi^*(x) \frac{d}{dx} (x \psi(x)) \\
 &= i \int_{-\infty}^{\infty} dx \psi^*(x) \left(1 + x \frac{d}{dx} \right) \psi(x) = \int_{-\infty}^{\infty} dx \psi^*(x) \left(i + ix \frac{d}{dx} \right) \psi(x)
 \end{aligned}$$

The boundary terms in the partial integration vanish as the wave function squared must vanish faster than $1/|x|$ at $\pm\infty$ to be normalizable. Comparing this to the definition $\langle \psi | \hat{M}^\dagger | \psi \rangle = \int_{-\infty}^{\infty} dx \psi^*(x) \hat{M}^\dagger \psi(x)$ which must hold for all possible wavefunctions ψ , we see that $\hat{M}^\dagger = i + ix \frac{d}{dx}$.

Grading: Partial credit of 2 points are given for writing down the relation $\langle \psi | \hat{M}^\dagger | \psi \rangle = \langle \psi | \hat{M} | \psi \rangle^*$. To get full score the correct answer must be derived in a convincing way.

Problem 2

2a)(2 points) A one dimensional harmonic oscillator with mass m and frequency ω is in the state

$$|\psi\rangle = \frac{1}{\sqrt{5}} (|0\rangle + 2i|2\rangle)$$

where $|n\rangle$ are energy eigenstates. The ladder operator

$$a \equiv \sqrt{\frac{m\omega}{2\hbar}} \left(x + \frac{i}{m\omega} p \right)$$

Calculate $a^\dagger |\psi\rangle$

Answer:

$$a^\dagger |\psi\rangle = \frac{1}{\sqrt{5}} (a^\dagger |0\rangle + 2ia^\dagger |2\rangle) = \frac{1}{\sqrt{5}} (|1\rangle + i2\sqrt{3}|3\rangle)$$

2b)(2 points) A one dimensional harmonic oscillator with mass m and frequency ω is in the state

$$|\psi(0)\rangle = \frac{1}{\sqrt{3}} (|0\rangle + i|1\rangle + |3\rangle)$$

at $t = 0$. Here $|n\rangle$ is an energy eigenstate with energy $E_n = \hbar\omega (n + 1/2)$.

What is the expectation value of the position operator x at time t ?

Answer: At time t the state is

$$|\psi(t)\rangle = \frac{1}{\sqrt{3}} (e^{-i\omega t/2}|0\rangle + ie^{-i3\omega t/2}|1\rangle + e^{-i7\omega t/2}|3\rangle)$$

The position operator $x = \sqrt{\frac{\hbar}{2m\omega}} (a + a^\dagger)$. Thus the expected value of the position operator at time t is

$$\begin{aligned} \langle\psi(t)|x|\psi(t)\rangle &= \sqrt{\frac{\hbar}{2m\omega}} \langle\psi(t)| (a + a^\dagger) |\psi(t)\rangle \\ &= \sqrt{\frac{\hbar}{2m\omega}} \langle\psi(t)| \frac{1}{\sqrt{3}} \left(e^{-i\omega t/2}|1\rangle + ie^{-i3\omega t/2} (\sqrt{2}|2\rangle + |0\rangle) + e^{-i7\omega t/2} (\sqrt{4}|4\rangle + \sqrt{3}|2\rangle) \right) \\ &= \sqrt{\frac{\hbar}{2m\omega}} \frac{1}{\sqrt{3}} (ie^{-i\omega t} - ie^{i\omega t}) = \sqrt{\frac{\hbar}{2m\omega}} \frac{1}{\sqrt{3}} (-i) (e^{i\omega t} - e^{-i\omega t}) \\ &= \sqrt{\frac{\hbar}{2m\omega}} \frac{1}{\sqrt{3}} (-i) 2i \sin(\omega t) = \underline{\sqrt{\frac{\hbar}{2m\omega}} \frac{2}{\sqrt{3}} \sin(\omega t)} \end{aligned}$$

2c)(2 points) The translation operator in one dimension that translates a function an amount a is defined as

$$\hat{T}f(x) = f(x + a)$$

The operator is unitary. The operator acts nontrivially, so it is not the identity operator. It is also clear that $\hat{T}^{-1}f(x) = f(x - a)$, thus $\hat{T}$ is not equal to its inverse. The hermitian conjugate $\hat{T}^\dagger$ satisfies:

$$\begin{aligned} \int dx f^*(x) \hat{T}^\dagger g(x) &= \left[\int dx g^*(x) \hat{T} f(x) \right]^* = \int dx g(x) f^*(x + a) = \int dx f^*(x) g(x - a) \\ &= \int dx f^*(x) \hat{T}^{-1} g(x) \implies \hat{T}^\dagger = \hat{T}^{-1}, \quad \underline{\hat{T} \text{ is unitary}} \end{aligned}$$

Since $\hat{T}^\dagger \neq \hat{T}$, the operator is not hermitian.

2d)(2 points) A spin-1/2 degree of freedom is in the state

$$|\psi\rangle = \frac{1}{\sqrt{5}} (|\uparrow\rangle - 2i|\downarrow\rangle)$$

where $|\uparrow\rangle$ and $|\downarrow\rangle$ are the eigenstates of the spin operator in the z -direction.

What is the probability to measure its spin- x component to be $+\hbar/2$?

Answer: The spin-x eigenstate with eigenvalue $+\hbar/2$ is $\frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$. Thus the probability to measure this value is

$$|\frac{1}{\sqrt{2}} \langle \uparrow | + \langle \downarrow | \rangle |\psi\rangle|^2 = |\frac{1}{\sqrt{2}} \frac{1}{\sqrt{5}} (1 - 2i)|^2 = \frac{1}{10} (1 - 2i)(1 + 2i) = \underline{\underline{\frac{1}{2}}}$$

2e)(2 points) A nucleus X with spin-3/2 is at rest. It decays into two other nuclei: a spin-1/2 nucleus A and a spin-1 nucleus B. The angular momentum after the decay is thus the spin of A, the spin of B and their (relative) orbital angular momentum. What are possible values of the (relative) orbital angular momentum for the decay products A and B? Assume that the total angular momentum is conserved in the decay process.

Answer: The total angular momentum before the decay is $j = 3/2$. After the decay the total angular momentum operator is the sum of the spins of the particles as well as their (relative) orbital angular momentum: $\vec{J} = \vec{S} + \vec{L}$. The total spin of the particles is $\vec{S} = \vec{S}_A + \vec{S}_B$ and $s_A = 1/2$ and $s_B = 1$ gives the following possible values for the total spin $s \in \{1/2, 3/2\}$. With a given value l for the relative orbital angular momentum the possible values for the total angular momentum after the decay is thus $j' \in \{|l - 3/2|, |l - 3/2| + 1, \dots, l + 3/2\}$. We see that for $l \in \{0, 1, 2, 3\}$ one of the allowed values is $j' = 3/2$, thus all of these values for l are allowed. For $l > 3$ $j' > 3/2$, so $l > 3$ is not possible.

2f)(2 points) Two particles, one with spin-1 and the other with spin-2, at rest are in a state with total spin 2 and total spin-z component +1.

What is the probability to measure the spin-2 particle to have spin-z component 0 in this state?

Answer: Inspecting the Clebsch-Gordan table 2×1 (Combining a spin-2 with a spin-1) one see that the state with total spin 2 and total spin-z component +1 is

$$|2, +1\rangle = \frac{1}{\sqrt{3}}|2, +2\rangle \otimes |1, -1\rangle + \frac{1}{\sqrt{6}}|2, +1\rangle \otimes |1, 0\rangle - \frac{1}{\sqrt{2}}|2, 0\rangle \otimes |1, +1\rangle$$

The probability to measure the spin-2 particle to have spin-z component 0 is found by

computing

$$\langle 2, +1 | \left(|2, 0\rangle \langle 2, 0| \otimes I \right) |2, +1\rangle = \underline{\underline{\frac{1}{2}}}$$

2g)(2 points) A certain material has 4 electrons per atomic nucleus that are free to move around in the material (i.e. they are not bound to a particular nucleus).

From the band theory picture, where electron-electron interactions are neglected, this material is predicted to be

Answer: There are $2N$ available one-particle states in a band built out of a periodic lattice of N potential wells. With N nuclei and $4N$ electrons that are free to move around in the crystal, exactly two bands are fully filled. The band theory picture therefore predicts that the material is an insulator or a semiconductor as there will be an energy gap to any excitations. Grading: Full score, 2 points, are given for selecting *either insulator, semiconductor, or both*. The size of the band gap was not given, so one cannot strictly conclude that band theory predicts a semiconductor (a semiconductor is however always insulating), however those who ticked off semiconductor will not be penalized.

2h)(2 points) The second order perturbative correction to the ground state energy is always....?

Answer: The expression for the second order perturbative correction to the ground state energy is

$$E_0^2 = \sum_{m \neq 0} \frac{|\langle m | H^1 | 0 \rangle|^2}{E_0 - E_m}$$

The numerator is always positive and since the denominator $E_m \geq E_0$, the second order perturbative correction is always negative.

2i)(2 points) Hydrogen atoms in the ground state $|100\rangle$ are exposed to an oscillating linearly polarized electric field with polarization in the z-direction. The field induces electric dipole transitions to the state $|310\rangle$ with a transition rate R .

If the electric field polarization is changed to the x-direction, what will the electric dipole transition rate to $|310\rangle$ be?

Answer: In the electric dipole approximation the transition rate is proportional to $|\vec{E} \cdot \langle 310 | \vec{r} | 100 \rangle|^2$. Because $|310\rangle$ and $|100\rangle$ are both $m = 0$ states it follows that

$$\langle 310 | x | 100 \rangle = 0, \quad \langle 310 | y | 100 \rangle = 0, \quad \langle 310 | z | 100 \rangle \neq 0$$

So only the z-direction contributes to transitions. Therefore with the field parameterized as $\vec{E} = E_0 (\sin \theta \hat{e}_x + \cos \theta \hat{e}_z)$ the transition rate as a function of angle $R(\theta)$ is

$$R(\theta) \propto |\vec{E} \cdot \hat{e}_z|^2 = E_0^2 \cos^2(\theta)$$

So $R(\pi/4)/R(0) = \cos^2(\pi/4) = \frac{1}{2}$ which implies a transition rate $R/2$.

2j)(2 points) In the first Born approximation, the scattering *amplitude* is proportional to the matrix element of the interaction between the incoming and scattered particle. This matrix element has two parts, a spatial one which is the same in both cases, and a spin part. The spin matrix element is

$$\langle S_t | \vec{S}_A \cdot \vec{S}_B | S_t \rangle = \frac{1}{2} \langle S_t | \left(S_t(S_t + 1) - S_A(S_A + 1) - S_B(S_B + 1) \right) | S_t \rangle$$

where S_t is the value of the total spin, and $S_A = 1$, $S_B = 1/2$. The total cross section (and also the differential cross section) is proportional to the scattering amplitude *squared*. Thus

$$\frac{\sigma_{1/2}}{\sigma_{3/2}} = \left| \frac{\frac{1}{2} \left(\frac{3}{2} \right) - 2 - \frac{3}{4}}{\frac{3}{2} \left(\frac{5}{2} \right) - 2 - \frac{3}{4}} \right|^2 = \left| \frac{-2}{1} \right|^2 = \underline{4}$$

Problem 3

3a)(6 points) The $l = 1$ spherical harmonics are

$$Y_1^0(\theta, \phi) = \sqrt{\frac{3}{4\pi}} \cos \theta, \quad Y_1^{\pm 1}(\theta, \phi) = \mp \sqrt{\frac{3}{8\pi}} \sin \theta e^{\pm i\phi}$$

The action of R_x on these gives

$$R_x Y_1^0 = Y_1^0, \quad R_x Y_1^{\pm 1} = \mp \sqrt{\frac{3}{8\pi}} \sin \theta e^{\pm i(\pi - \phi)} = Y_1^{\mp 1}$$

We see that Y_1^0 is an eigenfunction of R_x with eigenvalue $+1$, while $Y_1^{\pm 1}$ are not eigenfunctions. However by adding and subtracting the equations

$$R_x Y_1^{+1} = Y_1^{-1}$$

$$R_x Y_1^{-1} = Y_1^{+1}$$

we find that the equal weighted linear combinations of these are eigenfunctions

$$\begin{aligned} R_x (Y_1^{+1} + Y_1^{-1}) &= + (Y_1^{+1} + Y_1^{-1}) \\ R_x (Y_1^{+1} - Y_1^{-1}) &= - (Y_1^{+1} - Y_1^{-1}) \end{aligned}$$

thus $\frac{1}{\sqrt{2}} (Y_1^{+1} + Y_1^{-1})$ has eigenvalue $+1$ and $\frac{1}{\sqrt{2}} (Y_1^{+1} - Y_1^{-1})$ has eigenvalue -1 . Using the fact that $2 \cos \phi = (e^{i\phi} + e^{-i\phi})$ and $2i \sin \phi = (e^{i\phi} - e^{-i\phi})$ these eigenfunctions can be written

$$\begin{aligned} \frac{1}{\sqrt{2}} (Y_1^{+1} + Y_1^{-1}) &= \sqrt{\frac{3}{16\pi}} \sin \theta (-e^{i\phi} + e^{-i\phi}) = -i \sqrt{\frac{3}{4\pi}} \sin \theta \sin \phi = -i \sqrt{\frac{3}{4\pi}} \frac{y}{r} \\ \frac{1}{\sqrt{2}} (Y_1^{+1} - Y_1^{-1}) &= \sqrt{\frac{3}{16\pi}} \sin \theta (-e^{i\phi} - e^{-i\phi}) = -\sqrt{\frac{3}{4\pi}} \sin \theta \cos \phi = -\sqrt{\frac{3}{4\pi}} \frac{x}{r} \\ Y_1^0 &= \sqrt{\frac{3}{4\pi}} \cos \theta = \sqrt{\frac{3}{4\pi}} \frac{z}{r} \end{aligned}$$

With this rewriting we see immediately that these eigenfunctions are also eigenfunctions of R_y and R_z , because all these operators do is to change the sign of one of the cartesian coordinate components. We are free to multiply the eigenfunctions by a phase factors. Thus writing the eigenvalues as a set $\{R_x, R_y, R_z\}$ we can summarize the eigenvectors and eigenvalues as

$$\begin{aligned} Y_1^x &\equiv \sqrt{\frac{3}{4\pi}} \frac{x}{r} = \frac{1}{\sqrt{2}} (Y_1^{-1} - Y_1^1) & \{-1, +1, +1\} \\ Y_1^y &\equiv \sqrt{\frac{3}{4\pi}} \frac{y}{r} = \frac{i}{\sqrt{2}} (Y_1^{-1} + Y_1^1) & \{+1, -1, -1\} \\ Y_1^z &\equiv \sqrt{\frac{3}{4\pi}} \frac{z}{r} = Y_1^0 & \{+1, +1, -1\} \end{aligned}$$

Grading: Partial credit, 2 points, are given for realizing that the linear combinations $Y_1^1 \pm Y_1^{-1}$ are eigenfunctions of R_x and R_y . Also 1 point is given for realizing that all the eigenvalues are ± 1 , and 1 point for realizing that Y_1^0 is an eigenfunction of R_z with eigenvalue -1 . For full score, all the eigenfunctions with corresponding eigenvalues must be listed.

3b)(6 points) The $n = 2$ level of the Coulomb-problem has the following four degenerate energy kets $|200\rangle, |210\rangle, |21 \pm 1\rangle$ represented in the position representation by the functions

$$\psi_{200} = R_{20}(r)Y_0^0(\theta, \phi), \quad \psi_{210} = R_{21}(r)Y_1^0(\theta, \phi), \quad \psi_{21\pm 1} = R_{21}(r)Y_1^{\pm 1}(\theta, \phi)$$

where

$$R_{20}(r) = \frac{1}{\sqrt{2a^3}} \left(1 - \frac{r}{2a}\right) e^{-r/2a}, \quad R_{21}(r) = \frac{1}{\sqrt{24a^3}} \frac{r}{a} e^{-r/2a}.$$

The good states diagonalize the perturbation in the subspace of the degenerate states. Since the perturbation V is not dependent on ϕ , only matrix elements between states with the same m quantum number is non-zero. Therefore the only possibly finite off-diagonal matrix element is

$$\langle 200|V|210\rangle = \alpha \int dV \frac{1}{\sqrt{4\pi}} R_{20}(r) R_{21}(r) (3z^2 - r^2) \sqrt{\frac{3}{4\pi}} \frac{z}{r}$$

where we have written $\cos\theta = z/r$. However this integral is also in fact *zero* since the integrand is odd in z . Thus the four original states $|200\rangle, |210\rangle, |21 \pm 1\rangle$ diagonalize the perturbation, and are therefore good states.

An alternative way to solve this problem is to search for an operator which commutes with the Hamiltonian and the perturbation. From the problem text it is reasonable to guess that one can use the reflection operators. The perturbation $V(\vec{r})$ is even under any of the reflection operators which means that

$$R_x V R_x f(x, y, z) = R_x V(x, y, z) f(-x, y, z) = V(-x, y, z) f(x, y, z) = V(x, y, z) f(x, y, z)$$

Thus $R_x V R_x = V$ and since $R_x = R_x^{-1}$ we have $[R_x, V] = 0$. The same holds for the other reflection operators. The same argument can be used to show that the reflection operators also commute with H . Thus we can construct for instance the operator

$$R = \frac{1}{2} \left[(1 - R_x) + 2(1 - R_y) + 3(1 - R_z) \right]$$

This operator is hermitian and commutes with both H and V . The eigenfunctions of this operator are eigenfunctions of the three reflection operators. And those belonging to the $l = 1$ subspace were found in 3a). In addition the state $|200\rangle$ is also an eigenfunction. Thus we see that the eigenvalues of these four states are different as only the eigenvalue -1 contributes. Thus R has eigenvalue +1 for the x -function, +2 for the y -function and +3 for the z -function. We also note that for the fully spherically symmetric function ($|200\rangle$) the eigenvalue of R is 0. According to the theorem 7.2.2 in Griffiths, the good states are therefore the eigenstates of the reflection operators multiplied by the appropriate radial part which does not change under reflection:

$$\psi_0 = \psi_{200} = R_{20}(r) \frac{1}{\sqrt{4\pi}}, \quad \psi_x = R_{21}(r) \sqrt{\frac{3}{4\pi}} \frac{x}{r}, \quad \psi_y = R_{21}(r) \sqrt{\frac{3}{4\pi}} \frac{y}{r}, \quad \psi_z = R_{21}(r) \sqrt{\frac{3}{4\pi}} \frac{z}{r}$$

We note that these good states are slightly different from what found above as $\psi_{21\pm1} = \frac{1}{\sqrt{2}}(\psi_x \pm i\psi_y)$. Thus the good states of this problem are not unique, which is an indication that the degeneracy will not be completely lifted by the perturbation V . For instance by considering other symmetry operators, like for instance a 90 degree rotation in the xy -plane (which also commutes with H and V), and the reflection operator R_z we would have found the “original” set of good states.

Therefore the “general” set of good states in this problem are $|200\rangle, |210\rangle$ and two orthogonal linear combinations of $|21-1\rangle$ and $|21+1\rangle$.

Grading: Full score will be given if good states are found correctly. If the good states are not found, partial credit is given for using symmetry arguments correctly to find operators on the form R or similar. Also 1 point is awarded for mentioning that only matrix elements between states with the same m quantum value can be non-zero. 1 point is given for stating that the good states diagonalize the perturbation matrix. Also 1 point is given for listing correctly all the four degenerate unperturbed states.

3c)(6 points) The first order energy splittings can be solved straightforwardly by writing down the 4x4-matrix of the perturbation sandwiched between the energy eigenstates of the $n = 2$ level. The four degenerate states of the unperturbed problem are

$$\begin{aligned}\psi_{200} &= R_{20}(r)Y_0^0(\theta, \phi) = R_{20}(r)\frac{1}{\sqrt{4\pi}} \\ \psi_{210} &= R_{21}(r)Y_1^0(\theta, \phi) = R_{21}(r)\sqrt{\frac{3}{4\pi}}\frac{z}{r} \\ \psi_{21\pm1} &= R_{21}(r)Y_1^{\pm1}(\theta, \phi) = \mp R_{21}(r)\sqrt{\frac{3}{8\pi}}\frac{x \pm iy}{r}\end{aligned}$$

where we have used $\sin\theta e^{\pm i\phi} = \sin\theta(\cos\phi \pm i\sin\phi) = (x \pm iy)/r$. We must compute the matrix elements of the perturbation V between all these states. Since V does not involve ϕ it is clear that only matrix elements between states with the same m values will be non-zero. Also since V is even in x, y , and z , integrals with integrands that are odd in either x, y or z will be zero. Therefore the matrix is diagonal and the diagonal matrix elements are:

$$\langle 200|V|200\rangle = \frac{\alpha}{4\pi} \int dV R_{20}^2(r) (3z^2 - r^2) = \frac{\alpha}{4\pi} \int dV R_{20}^2(r) \left(3\frac{1}{3} - 1\right) r^2 = 0$$

where we used the integral identity $\int dV z^2 f(r) = \int dV \frac{1}{3} r^2 f(r)$. The second diagonal matrix

element is

$$\langle 210|V|210\rangle = \frac{3\alpha}{4\pi} \int dV R_{21}^2(r) (3z^2 - r^2) \frac{z^2}{r^2} = \alpha \int dV \left(3\frac{1}{5} - \frac{1}{3}\right) r^4 g(r) = \frac{4}{15}\alpha \int dV r^4 g(r)$$

where we have used the integral identities in the problem text and introduced the spherically symmetric function $g(r) = \frac{3}{4\pi} R_{21}^2 \frac{1}{r^2} = \frac{1}{32\pi a^5} e^{-r/a}$. The integral is

$$\int dV r^4 g(r) = 4\pi \frac{1}{32\pi a^5} \int_0^\infty dr r^6 e^{-r/a} = \frac{4\pi}{32\pi a^5} a^7 \int_0^\infty dx x^6 e^{-x} = \frac{4\pi}{32\pi} a^2 6! = 90a^2$$

which gives

$$\langle 210|V|210\rangle = \alpha \frac{4}{15} 90a^2 = 24\alpha a^2$$

The remaining two diagonal matrix elements are

$$\begin{aligned} \langle 21 \pm 1|V|21 \pm 1\rangle &= \frac{3\alpha}{8\pi} \int dV R_{21}^2(r) (3z^2 - r^2) \frac{x^2 + y^2}{r^2} \\ &= \frac{3\alpha}{8\pi} \int dV R_{21}^2(r) (3z^2 - r^2) \frac{x^2 + y^2 + z^2 - z^2}{r^2} \\ &= -\frac{3\alpha}{8\pi} \int dV R_{21}^2(r) (3z^2 - r^2) \frac{z^2}{r^2} = -\frac{1}{2} \langle 210|V|210\rangle = -12\alpha a^2 \end{aligned}$$

where we have used $r^2 = x^2 + y^2 + z^2$ and the first integral identity in the problem text. Thus the perturbation matrix is diagonal, consistent with the good states found in 3b), and so the energy corrections are: $0, 24\alpha a^2, -12\alpha a^2, -12\alpha a^2$.

Alternatively one can use the other set of good states found in 3b). Then

$$E_0^1 = \alpha \int dV (3z^2 - r^2) |\psi_0|^2 = \alpha \int dV \left(3\frac{1}{3}r^2 - r^2\right) |\psi_0|^2 = 0$$

where we have used the fact that ψ_0 is a function of r only, and the integral identity $\int dV z^2 f(r) = \int dV \frac{1}{3} r^2 f(r)$. The other energy corrections can be written

$$\begin{aligned} E_x^1 &= \alpha \int dV (3z^2 - r^2) |\psi_x|^2 = \alpha \int dV (3z^2 - r^2) x^2 g(r) \\ E_y^1 &= \alpha \int dV (3z^2 - r^2) |\psi_y|^2 = \alpha \int dV (3z^2 - r^2) y^2 g(r) \\ E_z^1 &= \alpha \int dV (3z^2 - r^2) |\psi_z|^2 = \alpha \int dV (3z^2 - r^2) z^2 g(r) \end{aligned}$$

where the spherically symmetric function $g(r) = \frac{3}{4\pi} R_{21}^2 \frac{1}{r^2} = \frac{1}{32\pi a^5} e^{-r/a}$. Using the integral

identities given in the problem text, we get

$$\begin{aligned} E_x^1 &= \alpha \int dV \left(3\frac{1}{15} - \frac{1}{3} \right) r^4 g(r) = -\alpha \frac{2}{15} \int dV r^4 g(r) \\ E_y^1 &= \alpha \int dV \left(3\frac{1}{15} - \frac{1}{3} \right) r^4 g(r) = -\alpha \frac{2}{15} \int dV r^4 g(r) \\ E_z^1 &= \alpha \int dV \left(3\frac{1}{5} - \frac{1}{3} \right) r^4 g(r) = \alpha \frac{4}{15} \int dV r^4 g(r) \end{aligned}$$

The integral

$$\int dV r^4 g(r) = 4\pi \frac{1}{32\pi a^5} \int_0^\infty dr r^6 e^{-r/a} = \frac{4\pi}{32\pi a^5} a^7 \int_0^\infty dx x^6 e^{-x} = \frac{4\pi}{32\pi} a^2 6! = 90a^2$$

which gives the following energies $E_0 = 0$, $E_x = -12\alpha a_0^2$, $E_y = -12\alpha a_0^2$ and $E_z = +24\alpha a_0^2$, the same as in the previous approach.

Thus the $n = 2$ level splits into 3 distinct energy levels, one of them is two-fold degenerate and is the lowest energy for $\alpha > 0$ and the highest for $\alpha < 0$, see Figure.

Comment: This V occurs in tetragonal crystals where one of the crystal axis is longer (or shorter) than the other two. The fact that there is a remnant symmetry as two of the crystal directions in a tetragonal crystal are still equivalent leads to the remaining degeneracy found in this problem.



Figure 1: Energy level diagrams.

Grading: To get full score, the energy corrections and energy level diagrams must be correct. Partial score is given if some of the matrix elements are calculated correctly. Also, if no calculations were performed, half a point is awarded for stating $E^1 = \langle \psi | V | \psi \rangle$.

4a)(6 points) The potential is spherically symmetric so the angular dependence of the wavefunctions are described by the spherical harmonics. Inside the potential $r < a$, the s-wave ($l = 0$) radial equation for $u \equiv rR(r)$ is

$$\frac{d^2 u}{dr^2} - \left(0 + \frac{2m}{\hbar^2} V_0 \right) u = -k^2 u \implies \frac{d^2 u}{dr^2} = k'^2 u$$

where we have defined $k'^2 = \frac{2m}{\hbar^2}V_0 - k^2 > 0$ for $E < V_0$. The general solution of this equation is

$$u(r) = A \sinh(k'r) + B \cosh(k'r)$$

This must vanish at $r \rightarrow 0$, thus $B = 0$ and the inside solution becomes

$$u(r) = A \sinh(k'r), \quad r < a$$

The general outside ($r > a$) solution is given in Griffiths Eq. (10.29). Extrating its s-wave part one finds

$$u(r) = rA' \left(j_0(kr) + ika_0 h_0^1(kr) \right)$$

where we have used $P_0(\cos \theta) = 1$. Using the definition of the Hankel function $h_0^1(kr) = j_0(kr) + in_0(kr)$ and expressing a_0 in terms of phase shifts: $a_0 = \frac{1}{k}e^{i\delta_0} \sin \delta_0$ (Griffiths Eq. (10.46)), this can be rewritten as

$$\begin{aligned} u(r) &= rA' \left(j_0(kr) + ie^{i\delta_0} \sin \delta_0 (j_0(kr) + in_0(kr)) \right) \\ &= rA' \left((1 + ie^{i\delta_0} \sin \delta_0) j_0(kr) - e^{i\delta_0} \sin \delta_0 n_0(kr) \right) \end{aligned}$$

Now, as shown in the lectures, we can rewrite $1 + ie^{i\delta_0} \sin \delta_0 = 1 + ie^{i\delta_0} \frac{1}{2i} (e^{i\delta_0} - e^{-i\delta_0}) = \frac{1}{2} + \frac{e^{i2\delta_0}}{2} = e^{i\delta_0} \cos \delta_0$ and so

$$u(r) = rA'e^{i\delta_0} \left(\sin \delta_0 j_0(kr) - \cos(\delta_0) n_0(kr) \right)$$

Using the relations $j_0(kr) = \sin(kr)/kr$ and $n_0(kr) = -\cos(kr)/kr$ this can be further rewritten as

$$u(r) = A' \frac{e^{i\delta_0}}{k} (\sin \delta_0 \cos(kr) + \cos(\delta_0) \sin(kr)) = A' \frac{e^{i\delta_0}}{k} \sin(\delta_0 + kr)$$

The inside and outside solutions must match at $r = a$ and so must their derivatives. This gives the equations

$$\begin{aligned} A \sinh(k'a) &= \frac{A'e^{i\delta_0}}{k} \sin(\delta_0 + ka) \\ Ak' \cosh(k'a) &= \frac{A'e^{i\delta_0}}{k} k \cos(\delta_0 + ka) \end{aligned}$$

dividing these equations by each other, we get

$$\frac{1}{k'} \tanh(k'a) = \frac{1}{k} \tan(\delta_0 + ka) \implies \tan(\delta_0 + ka) = \frac{k}{k'} \tanh(k'a)$$

or

$$\delta_0 = \arctan \left(\frac{k}{k'} \tanh(k'a) \right) - ka$$

The expression for the s-wave part of the total cross section is

$$\sigma_{l=0} = \frac{4\pi}{k^2} \sin^2 \delta_0$$

When $V_0 \gg E = \frac{\hbar^2 k^2}{2m}$ we can set $\frac{\hbar^2 k'^2}{2m} \approx V_0$, and the ratio $k/k' \simeq \sqrt{E/V_0} \ll 1$. Since $-1 < \tanh x < 1$ the argument of arctan is therefore small, and we may expand it using $\arctan x = x + \dots$ giving

$$\delta_0 = -ka \left(1 - \frac{\tanh(k'a)}{k'a} + \dots \right)$$

In the long wavelength limit $ka \ll 1$ the phase shift δ_0 is small, thus we can approximate $\sin \delta_0 = \delta_0$. Therefore the s-wave part of the total scattering cross section becomes

$$\sigma_{l=0} \approx \frac{4\pi}{k^2} (ka)^2 \left(1 - \frac{\tanh(k'a)}{k'a} \right)^2 = 4\pi a^2 \left(1 - \frac{\tanh(k'a)}{k'a} \right)^2 \approx 4\pi a^2 \left(1 - \frac{2}{k'a} \right)$$

where in the last equality we have expanded the result for large V_0 or equivalently large $k'a$ using $\tanh k'a \approx 1$ and $(1 - \frac{1}{x})^2 \approx 1 - \frac{2}{x}$. For $V_0 \rightarrow \infty$, $(k'a \rightarrow \infty)$, we recover the hard sphere scattering result $4\pi a^2$. The leading order correction to this is

$$-4\pi a^2 \frac{2}{k'a} = -8\pi a^2 \sqrt{\frac{\hbar^2}{2ma^2 V_0}}$$

Grading: The correct s-wave phase shift gives in total 4 points. 2 points are awarded for the correct long wavelength analysis. Partial credit is generally awarded for how far towards the answers one gets. In particular the expression for k' is awarded 1 point, good attempts to connect the inside and outside wave functions, 1-2 points. No points are awarded for just writing down general formulae like for instance the scattering cross section expressed in terms of the phase shift.