Qualifying Exam
Quantum Mechanics – SOLUTIONS
August 2020

Solve one of the two problems in Part A, and one of the two problems in Part B.
Each problem is worth 50 points.

Part A

Problem 1.
Let us consider an electron whose squared orbital angular momentum $\mathbf{L}^2$ is measured to be $6\hbar^2$.

1.a) **[5 points] For each one of the two bases described above, list all the possible states for the electron which are compatible with this measurement.**

We have $s = \frac{1}{2}$ and $l = 2$ (since $l(l+1) = 6$). Since $l + s \leq j \leq |l - s|$, the allowed values for j will be $j = \frac{5}{2}$, $j = \frac{3}{2}$.

As a consequence, there will be ten possible states in the basis $\{|jm_j\rangle\}$: $j = \frac{5}{2}$ with $m_j = \frac{5}{2}, \frac{3}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{3}{2}, -\frac{5}{2}$ (six states) and $j = \frac{3}{2}$ with $m_j = \frac{3}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{3}{2}$ (four states).

In the basis $\{|m_l m_s\rangle\}$, we can have all possible combinations of $m_s = -\frac{1}{2}, \frac{1}{2}$ with $m_l = 2, 1, 0, -1, -2$, which is again ten states.

1.b) **[15 points] Find the expression of the following basis states $\{|jm_j\rangle\}$ in terms of the appropriate elements of the basis $\{|m_l m_s\rangle\}$.**

1.b.1 : First state on the ladder, here is only one possible way of satisfying $m_j = m_s + m_l$, therefore

$$|j = \frac{5}{2}\ m_j = \frac{5}{2}\rangle = |m_l = 2\ m_s = \frac{1}{2}\rangle$$

1.b.2 : We should apply the lowering operator on both sides to obtain

$$|j = \frac{5}{2}\ m_j = \frac{3}{2}\rangle = \sqrt{\frac{4}{5}}\ |m_l = 1\ m_s = \frac{1}{2}\rangle + \sqrt{\frac{1}{5}}\ |m_l = 2\ m_s = -\frac{1}{2}\rangle$$

and then apply the orthogonality condition to get

$$|j = \frac{3}{2}\ m_j = \frac{3}{2}\rangle = \sqrt{\frac{1}{5}}\ |m_l = 1\ m_s = \frac{1}{2}\rangle - \sqrt{\frac{4}{5}}\ |m_l = 2\ m_s = -\frac{1}{2}\rangle$$

1.b.3 : Not a possible state. We cannot have $j = \frac{1}{2}$ if $s = \frac{1}{2}$ and $l = 2$.

1.b.4 : We can continue to apply the lowering operator until we reach the minimum of m_j, or start from the bottom of the ladder (which is faster). The only combination of m_s and m_l that allows for $m_j = -\frac{5}{2}$ is

$$|j = \frac{5}{2}\ m_j = -\frac{5}{2}\rangle = |m_l = -2\ m_s = -\frac{1}{2}\rangle$$

1.c) **[15 points] Now assume the electron to be in the state with $j = \frac{3}{2}$, and $m_j = \frac{1}{2}$ (and the value of l is the same as in the previous questions). If one measures the z-components of the electron orbital angular momentum and spin, what are the possible values and their probabilities?**

In our problem, there are only two configurations of m_s and m_l that are compatible with $|j = \frac{3}{2}$, and $m_j = \frac{1}{2}$, namely the states $|m_l = 1\ m_s = -\frac{1}{2}\rangle$ and $|m_l = 0\ m_s = \frac{1}{2}\rangle$.

To obtain the probabilities, we start from the expression that we obtained in question 1.b.2), and we apply once more the lowering operator, to obtain:

$$|j = \frac{3}{2}\ m_j = \frac{1}{2}\rangle = \sqrt{\frac{2}{5}}\ |m_l = 0\ m_s = \frac{1}{2}\rangle - \sqrt{\frac{3}{5}}\ |m_l = 1\ m_s = -\frac{1}{2}\rangle$$

which allows to read the probabilities $\frac{2}{5}$ and $\frac{3}{5}$, respectively for the pair of values $(m_l = 0, m_s = \frac{1}{2})$ and $(m_l = 1, m_s = -\frac{1}{2})$.

1.d) **[15 points] Let us now assume that the electron is in the state with $m_l = 1$ and $m_s = -\frac{1}{2}$ (again, l did not change). What are the possible values of j and their probabilities?**

Here we have the "inverse" problem as 1.c). The state $|m_l = 1 m_s = -\frac{1}{2}\rangle$ must be a linear combination of the states $|j = \frac{3}{2}\ m_j = \frac{1}{2}\rangle$ (which we know already) and $|j = \frac{5}{2}\ m_j = \frac{1}{2}\rangle$ (which we do not have yet).

Let us first find $|j = \frac{5}{2}\ m_j = \frac{1}{2}\rangle$. We can obtain it by applying the lowering operator to $|j = \frac{5}{2}\ m_j = \frac{3}{2}\rangle$ or simply by using the orthogonality with $|j = \frac{3}{2}\ m_j = \frac{1}{2}\rangle$. In either way, we get:

$$|j = \frac{5}{2}\ m_j = \frac{1}{2}\rangle = \sqrt{\frac{3}{5}}\ |m_l = 0\ m_s = \frac{1}{2}\rangle + \sqrt{\frac{2}{5}}\ |m_l = 1\ m_s = -\frac{1}{2}\rangle$$

We can solve now for $|m_l = 1\ m_s = -\frac{1}{2}\rangle$, to get

$$|m_l = 1\ m_s = -\frac{1}{2}\rangle = \sqrt{\frac{2}{5}}\ |j = \frac{5}{2}\ m_j = \frac{1}{2}\rangle - \sqrt{\frac{3}{5}}\ |j = \frac{3}{2}\ m_j = \frac{1}{2}\rangle$$

. Therefor, we will have $j = \frac{5}{2}$ with probability $\frac{2}{5}$ and $j = \frac{3}{2}$ with probability $\frac{3}{5}$.

Problem 2.
We want to study the problem of a particle approaching a one-dimensional asymmetric step potential, as described by the Hamiltonian $H = \frac{p^2}{2m} + V(x)$, where

$$V(x) = \begin{cases} 0 & -\infty \leq x \leq 0 \\ V_0 & 0 < x < a \\ V_1 & a \leq x \leq \infty \end{cases} .$$

Assume the energy of the particle to be $E > V_0 > V_1$.

2.a) [**5 points**] **Write the general form of the wave function in the three regions defined by the different values of** $V(x)$.

Region I $(-\infty \leq x \leq 0)$: $\Psi_I(x) = A\exp(ikx) + B\exp(-ikx)$ where $k = \frac{\sqrt{2mE}}{\hbar}$

Region II $(0 < x < a)$: $\Psi_{II}(x) = C\exp(ik_0x) + C\exp(-ik_0x)$ where $k_0 = \frac{\sqrt{2m(E-V_0)}}{\hbar}$

Region III $(a \leq x \leq \infty)$: $\Psi_{III}(x) = E\exp(ik_1x)$ where $k_1 = \frac{\sqrt{2m(E-V_1)}}{\hbar}$

Note that some students might choose the notation $A \to 1$, $B \to r$, and $E \to t$, which is a common notation in many textbooks (where r and t are called reflection and transmission coefficients).

2.b) [**5 points**] **What are the boundary conditions for the wave function at the points** $x = 0$ **and** $x = a$**?**

Impose the continuity of the wave function and its first derivative at $x = 0$ and $x = a$ (four conditions altogether).

$$A + B = C + D \tag{1}$$
$$k(A - B) = k_0(C - D) \tag{2}$$
$$C\exp(ik_0a) + D\exp(-ik_0a) = E\exp(ik_1a) \tag{3}$$
$$k_0C\exp(ik_0a) - k_0D\exp(-ik_0a) = k_1E\exp(ik_1a) \tag{4}$$

2.c) [**5 points**] **Using the fact that the probability current is constant, derive the relation between the transmission and reflection probabilities** T **and** R.

Using the relation for the probability current (given in the formulas):

$$j(x) = \text{Re}\left\{\frac{-i\hbar}{m}\ {}^*(x)\frac{\partial\psi(x)}{\partial x}\right\}$$

we can find:

$$j_I(x) = \frac{\hbar k}{m}\left(|A|^2 - |B|^2\right),\ j_{II}(x) = \frac{\hbar k_0}{m}\left(|C|^2 - |D|^2\right),\ j_{III}(x) = \frac{\hbar k_1}{m}|E|^2$$

and therefore, using the equality between $j_I(x)$ and $j_{III}(x)$:

$$k\left(|A|^2 - |B|^2\right) = k_1|E|^2$$

. Dividing both sides by $k|A|^2$ we get:

$$1 - \left|\frac{B}{A}\right|^2 = \frac{k_1}{k}\left|\frac{E}{A}\right|^2$$

That allows for the identifications of $T = \frac{k_1}{k}\left|\frac{E}{A}\right|^2$ and $R = \left|\frac{B}{A}\right|^2$, as transmission and reflection probabilities, respectively.

2.d) **[25 points] Use the relations that you derived in part 2.b) and 2.c) to compute the transmission probability T.**

Write C and D in terms of E, using the third and fourth equations.

$$C = \frac{k_0 - k_1}{2k_0}\exp\left[i(k_1 - k_0)a\right]\, E$$

$$D = \frac{k_0 + k_1}{2k_0}\exp\left[i(k_1 + k_0)a\right]\, E$$

The substitute in the first and second one to write A and B as functions of E. This allows to obtain:

$$2kA = (k + k_0)C + (k - k_0)D$$

$$A = \frac{k + k_0}{2k}\frac{k_1 - k_0}{2k_0}\exp\left[i(k_1 - k_0)a\right]\, E + \frac{k - k_0}{2k}\frac{k_1 + k_0}{2k_0}\exp\left[i(k_1 + k_0)a\right]\, E$$

$$\frac{A}{E} = \frac{\exp\left[ik_1 a\right]}{4kk_0}\left\{(k + k_0)(k_1 - k_0)\exp\left[-ik_0 a\right] + (k - k_0)(k_1 + k_0)\exp\left[ik_0 a\right]\,\right\}$$

$$\frac{A}{E} = \frac{\exp\left[ik_1 a\right]}{4kk_0}\left\{2\cos\left(k_0 a\right)\left(kk_0 + k_0 k_1\right) - 2i\sin\left(k_0 a\right)\left(k_0^2 + kk_1\right)\right\}$$

Then we can use

$$T = \frac{k_1}{k}\left|\frac{E}{A}\right|^2 = \frac{4\ k\ k_0^2\ k_1}{\cos^2\left(k_0 a\right)\left(kk_0 + k_0 k_1\right)^2 + \sin^2\left(k_0 a\right)\left(k_0^2 + kk_1\right)^2}$$

2.e) **[10 points] Check your solution for the transmission probability T in the limit $V_1 \to 0$. In this limit, your solution should reproduce the know value of T for the rectangular symmetric barrier, namely $T = \left[1 + \frac{V_0^2 \sin^2(k_0 a)}{4E(E - V_0)}\right]^{-1}$ where $k_0 = \frac{\sqrt{2m(E-V_0)}}{\hbar}$.**

This can be quite easily computed taking the limit $k_1 \to k$ in the expression above for T (note that k_0 is unchanged).

Formulas for Part A

Schrödinger Equation:

$i\hbar\frac{\partial\psi(x,t)}{\partial t} = \hat{H}\psi(x,t)\,,\quad \hat{H} = \frac{\hat{p}^2}{2m} + V(x)\,,\quad \hat{H}\psi_E(x) = E\psi_E(x)\,,$
$j(x) = \mathrm{Re}\left\{\frac{-i\hbar}{m}\psi^*(x)\frac{\partial\psi(x)}{\partial x}\right\}$

Angular Momentum Operators:

$[\hat{J}_x,\hat{J}_y] = i\hbar\hat{J}_z$ (or $[\hat{J}_i,\hat{J}_j] = i\hbar\epsilon_{ijk}\hat{J}_k$) , $[\hat{J}^2,\hat{J}_i] = 0$, $\hat{J}_\pm = \hat{J}_x \pm i\hat{J}_y$,
$\hat{J}_\pm|j\ m\rangle = \hbar\sqrt{j(j+1)-m(m\pm 1)}\ |j\ m\pm 1\rangle$

P.1

The WKB approximation is valuable in a wide range of systems that resemble the Schrödinger equation. Consider the Helmholtz equation in a one-dimensional optical cavity:

$$\left[\frac{d^2}{dx^2} + \varepsilon(x)k^2\right]\psi(x) = 0. \tag{1}$$

Here $\varepsilon(x)$ is the *real-valued* dielectric function and its frequency dependence is neglected. $k = \omega/c$ is the wave vector in free-space, where ω is the circular frequency and c is the speed of light in vacuum.

(I) Assume for now that k is real. Establish **one** connection between Eq. (1) and the time-independent Schrödinger equation. Point out what quatities play the roles of the mass, the potential and the energy. Note that there are multiple acceptable answers and take $\hbar = 1$.

Answer 1: The energy E is zero. $-\varepsilon(x)k^2$ is the potential (Note: the minus sign is required). $m = 0.5$.
Answer 2: The energy E is zero. $-\varepsilon(x)$ is the potential. $m = 0.5k^2$.
Answer 3: The energy E is k^2. $(1-\varepsilon(x))k^2$ is the potential. $m = 0.5$.
...

Here we consider a cavity of a finite size, i.e., $x \in [-L/2, L/2]$, and the refractive index $n(x) = \sqrt{\varepsilon(x)}$ is position-dependent inside the cavity but is a constant ($n_e > 0$) outside. Now we focus on the states that are defined by a solution of Eq. (1) with the incoming boundary condition $\psi(x,t) \propto e^{-in_e k|x|}$ in $|x| > L/2$. They correspond to the zeros of the scattering matrix.

(II) Write the boundary condition in terms of ψ'/ψ at $x = \pm L/2$ where $\psi' = d\psi/dx$.

Answer: $\psi'/\psi = -in_e k$ at $x = L/2$ and $in_e k$ at $x = -L/2$.

(III) Because of the incoming boundary condition, the system is no longer Hermitian and k is complex in general. Can you recover the WKB result learned in class using $\psi(x) = A(x)e^{i\phi(x)}$? Here $A(x)$, $\phi(x)$ are real.

Answer:

$$\psi' = (A' + iA\phi')e^{i\phi}, \qquad '' = (A'' + 2iA'\phi' + iA\phi'' - A(\phi')^2)e^{ik\phi} = -\varepsilon k^2 A e^{ik\phi}$$

By dropping A'', we find

$$i(2A'\phi' + A\phi'') = A((\phi')^2 - \varepsilon k^2).$$

Denoting $k^2 = f^2 + ig$ $(f, g \in \mathbb{R})$, we separate the real and imaginary part of the equation above:

$$2A'\phi' + A\phi'' = -A\varepsilon g, \quad 0 = (\phi')^2 - \varepsilon f^2.$$

The second equation above gives $\phi' = \pm\sqrt{\varepsilon f^2} \equiv \pm n(x) f$, similar to what we learned in class. However, the first equation needs more attention. We rewrite it as

$$(\ln\, y)' = \frac{y'}{y} = -\frac{g\phi'}{f^2},$$

where $y = A^2\phi' L$ is dimensionless. We then find $y \propto e^{-g\phi/f^2}$ and

$$A(x) \propto \frac{1}{\sqrt{n(x)}} e^{-g\phi/2f^2} \quad \to \quad (x) \propto \frac{1}{\sqrt{n(x)}} e^{i(1+ig/2f^2)\phi} = \frac{1}{\sqrt{n(x)}} e^{\pm i(f+ig/2f)\int dx\, n(x)}$$

Note that if we denote $k = k_r + ik_i$ and assume $0 < k_i \ll k_r$, we then find $f \approx k_r$ and $g = 2k_r k_i$. Therefore, the factor in the exponent is approximately k. If a student is unable to derive the result above, he has the option to start with a simpler ansatz in the next question.

(IV) How about using $\psi(x) = A(x)e^{ik\phi(x)}$? If it works, apply the WKB approximation using $A'' \approx 0$. Note that the result depends on whether $Re[k]$ vanishes.

Answer:

$$\psi' = (A' + ikA\phi')e^{ik\phi}, \qquad '' = (A'' + 2ikA'\phi' + ikA\phi'' - A(k\phi')^2)e^{ik\phi} = -\varepsilon k^2 Ae^{ik\phi}$$

By dropping A'', we find

$$i(2A'\phi' + A\phi'') = Ak((\phi')^2 - \varepsilon).$$

If k were real, then the derivation that follows would be exactly the same as in the Schrödinger equation. The imaginary part of k makes the result slightly different. Denoting again $k = k_r + ik_i$ ($k_{r,i} > 0$), we separate the real and imaginary part of the equation above:

$$2A'\phi' + A\phi'' = Ak_i((\phi')^2 - \varepsilon), \quad 0 = k_r((\phi')^2 - \varepsilon).$$

If $k_r \neq 0$, the second equation tells us that $\phi' = \pm\sqrt{\varepsilon} = \pm n(x)$, and the first equation indicates $A\phi' =$ const. The wave function is then given by

$$\psi(x) \propto \frac{1}{\sqrt{n(x)}} e^{ik\int n(x)dx},$$

which is again the same as in the Schrödinger equation. However, there exists zeros of the scattering matrix with $k_r = 0$ for some $\varepsilon(x)$, and we find $(\phi')^2 \neq \varepsilon$. As a result, the right hand side of $2A'\phi' + A\phi'' = Ak_i((\phi')^2 - \varepsilon)$ is not zero either. In other words, in this case the phase and amplitude of the wave function are not simply related.

(V) Assume $\varepsilon(x) = \varepsilon(-x)$, write down the wave function in the WKB approximation as sine and cosine functions. What is the argument of these sinusoidal functions?

Answer:

$$\psi_+(x) = \frac{1}{\sqrt{n(x)}} \cos\left(k\int_0^x n(x)dx\right) \quad \text{and} \quad \psi_-(x) = \frac{1}{\sqrt{n(x)}} \sin\left(k\int_0^x n(x)dx\right),$$

one for even-parity and the other for odd-parity. Check:

$$\psi_-(-x) = \frac{1}{\sqrt{n(x)}} \sin\left(k\int_0^{-x} n(x)dx\right) = \frac{1}{\sqrt{n(x)}} \sin\left(-k\int_0^{x} n(-x)dx\right) = -\psi_-(x).$$

We have used $x \to -x$ in the second step and $n(x) = n(-x)$ in the last step. Similarly, we find $\psi_+(-x) = \psi_+(x)$.

(VI) Using the boundary condition at either $x = L/2$ or $-L/2$, derive the analytical expressions satisfied by $k = k_r + ik_i$ ($k_{r,i} > 0$), one for even-parity and the other for odd-parity. Assuming $k_i \ll k_r$, analyze these express to show that they lead to the same form

$$k \approx \frac{1}{\bar{n}L}\left[q + i\ln\frac{2q}{|\alpha|}\right], \tag{2}$$

when $|\alpha| \ll q$. Specify the expressions for α, q, and the average refractive index $\bar{n}$ inside the cavity.

Answer: Using the boundary condition at $x = L/2$, we find

$$\left.\frac{\psi_-'}{\psi_-}\right|_{x=L/2} = \frac{\sqrt{n_e}[k\cos(z/2) - \frac{n'}{2n_e^2}\sin(z/2)]}{\frac{1}{\sqrt{n_e}}\sin(z/2)} = -in_e k, \quad \text{or} \quad \tan(z/2) = \frac{z}{-\alpha + iz},$$

where $z \equiv \bar{n}kL/2$ and $\alpha \equiv \bar{n}Ln'(x = L/2)/2n_e^2 \in \mathbb{R}$. $\bar{n}$ is the average of $n(x)$ inside the cavity, i.e., $\bar{n} = \int_{-L/2}^{L/2} n(x)dx/L$. Similarly, for the parity-even wave functions, we have

$$\tan(z/2) = \frac{\alpha - iz}{z}.$$

α is fixed, and at high energy we find $\delta \equiv |\alpha|/z \ll 1$. To the leading order of δ, we then find $e^{-iz} = \pm i\delta$, where "+" and "−" are for the two parities. Denoting $z = q + i\kappa$, we find $q \approx (m + 0.5)\pi$ $(m \in \mathbb{Z})$ by noting that e^{-iz} is approximately imaginary when $\delta \ll 1$. Finally, we derive Eq. (2) by taking the absolution value of e^{-iz} and the approximation $\delta \approx |\alpha|/q$, assuming $q \gg \kappa$.

P.2

(I) [15 pts] Consider a one-dimensional harmonic oscillator in the ground state $|0\rangle$ of the unperturbed Hamiltonian at $t = -\infty$. Let a perturbation $H_1(t) = Fxe^{-t^2/\tau^2}$ be applied between $t = -\infty$ and $+\infty$. Use the first-order time-dependent perturbation theory to calculate the probability that the oscillator is in the state $|n\rangle$ at $t = +\infty$.

Answer: Assuming $|\psi(t)\rangle = \sum_n d_n(t)e^{-iE_nt/\hbar}|n\rangle$ where the (shifted) energy levels are $E_n = n\hbar\omega$, we know

$$d_n(t) = \frac{-i}{\hbar}F\int_{-\infty}^{\infty}\langle n|x|0\rangle e^{-t^2/\tau^2}e^{in\omega t}dt. \tag{3}$$

In the midterm I tested the students about the selection rule based on the parity of the eigenstates. Here it is similar and we find only an odd $|n\rangle$ may have a nonzero transition probability. Furthermore, using $x = \sqrt{\hbar/2m\omega}(a + a^\dagger)$ and the Gaussian integral we find that only $d_1(+\infty)$ is nonzero:

$$d_1(+\infty) = \frac{-i}{\hbar}\sqrt{\frac{\hbar}{2m\omega}}F\tau\int_{-\infty}^{\infty}e^{-t^2}e^{i\omega\tau t}dt = iF\tau\left(\frac{\pi}{2m\hbar\omega}\right)^{1/2}e^{-\omega^2\tau^2/4}. \tag{4}$$

(II) [5 pts] Prove the adiabatic theorem using this example, i.e., if the Hamiltonian $H(t)$ is slowly varying, then a system starts out in $|n\rangle$ at $t = -\infty$ will end up in $|n\rangle$ again at $t = +\infty$. Show quantitatively how slow the variation needs to be in terms of the energy difference between two neighboring states.

Ansswer: We just need to show that $d_1(\infty) \to 0$, which requires $\omega\tau = \tau(E_1 - E_0)/\hbar \gg 1$ for a given ω.

(III) [15 pts] Now consider another case. If we start with a quantum bouncing ball in a box potential in one dimension and slowly modulate its length L with period τ, show that the requirement for the adiabatic theorem to hold is the same as in (II). Here we just need the order of magnitude estimation, and you may want to consider the wave-particle duality of the ball.

Answer: A reasonale condition for the adiabatic theorem to hold is the following: the time it takes for the ball to complete a round trip should be much shorther than τ. The energy of the nth level in a box potential is given by $n^2\hbar^2\pi^2/2mL^2$, and hence we estimate its momentum to be $p \sim \hbar/L$. The round-trip time is then $T = L/v = mL/p \sim mL^2/\hbar$. Note that $E_1 - E_0$ here is also on the order of $\hbar^2/mL^2$, so

$$T/\tau = mL^2/\hbar\tau = \hbar/(E_1 - E_0)\tau \ll 1, \tag{5}$$

which is the same condition as in (II).

(IV) The adiabatic theorem can also be verified by comparing time-dependent perturbation theory with time-independent perturbation theory. Let us come back to (II). At $t = 0$, does the time-dependent perturbation theory you have used give the same result as the time-independent perturbation theory to the first order in the adiabatic limit? What if $H_1(t) = Fxe^{t/\tau}$?

Answer: At $t = 0$, we find

$$d_1(0) = \frac{-i}{\hbar}\langle 1|Fx|0\rangle\tau \int_{-\infty}^{0} e^{-t^2} e^{i\omega\tau t} dt \equiv \frac{-i}{\hbar}\langle 1|Fx|0\rangle\tau I. \tag{6}$$

We observe that

$$I^* = \int_{-\infty}^{0} e^{-t^2} e^{-i\omega\tau t} dt = \int_{0}^{\infty} e^{-t^2} e^{i\omega\tau t} dt \tag{7}$$

and

$$I + I^* = \int_{-\infty}^{\infty} e^{-t^2} e^{i\omega\tau t} dt = \sqrt{\pi} e^{-\omega^2\tau^2/2}. \tag{8}$$

Therefore, the real part of I, as well as the imaginary part of $d_1(0) \propto \tau e^{-\omega^2\tau^2/2}$, vanishes in the limit that $\omega\tau \gg 1$ for a given ω. The imaginary part of I, on the other hand, is given by the error function, or equivalently, the Dawson integral:

$$\mathrm{Im}[I] = -D_+\left(\frac{\omega\tau}{2}\right) = -e^{-\omega^2\tau^2/4} \int_{0}^{\omega\tau/2} e^{y^2} dy = -\frac{1}{2}\sqrt{\pi} e^{-\omega^2\tau^2/4} \mathrm{erfi}(\omega\tau/2). \tag{9}$$

Using the property that $D_+(x) \approx (2x)^{-1}$ when $x \to +\infty$, we find

$$d_1(0) = -\frac{1}{\hbar\omega}\langle 1|Fx|0\rangle = \frac{\langle 1|H_1|0\rangle}{E_0 - E_1}, \tag{10}$$

which is what the time-independent perturbation theory gives us. Now for the new H_1, we have

$$d_1(0) = \frac{-i}{\hbar} \int_{-\infty}^{0} \langle 1|Fx|0\rangle e^{t/\tau} e^{in\omega t} dt = \frac{(-i/\hbar)\langle 1|Fx|0\rangle}{1/\tau + i\omega} \to -\frac{\langle 1|Fx|0\rangle}{\hbar\omega} = \frac{\langle 1|H_1|0\rangle}{E_0 - E_1}, \tag{11}$$

which again confirms the adiabatic theorem.

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Problem #1

a) We use: $[\hat{H}, \hat{a}] = -\hat{a} \Rightarrow \hat{H}\hat{a} = \hat{a}H - \hat{a}$

$[H, \hat{a}^+] = +\hat{a}^+ \Rightarrow \hat{H}\hat{a}^+ = a^+\hat{H} + \hat{a}^+$

Define $|\alpha\rangle = \hat{a}|n\rangle$

$$\boxed{\hat{H}|\alpha\rangle} = \hat{H}\hat{a}|n\rangle = (\hat{a}\hat{H} - \hat{a})|n\rangle = (E_n - 1)\hat{a}|n\rangle$$

$$= \boxed{(E_n - 1)|\alpha\rangle}$$

Similarly for $|\beta\rangle \Rightarrow \hat{H}|\beta\rangle = (E_n + 1)|\beta\rangle$.

b) Possible outcomes (AT ALL t) are:

$E_0 = \frac{1}{2}\hbar\omega$ with $P_0 = 1/4$

$E_3 = \frac{7}{2}\hbar\omega$ with $P_3 = 1/4$

$E_5 = \frac{11}{2}\hbar\omega$ with $P_5 = 1/2$

note that $\sum_i P_i = 1$

c) $\langle s|\hat{H}|s\rangle = \sum_n E_n P_n =$

$$= \left(\frac{1}{2}\frac{1}{4} + \frac{7}{2}\frac{1}{4} + \frac{11}{2}\frac{1}{2}\right)\hbar\omega$$

$$= \frac{1}{8}(1 + 7 + 22)\hbar\omega = \frac{30}{8}\hbar\omega = \boxed{\frac{15}{4}\hbar\omega}$$

$$\langle s|\hat{H}^2|s\rangle = \sum_n E_n^2 P_n = \ldots = \frac{73}{4}\hbar^2\omega^2$$

$$(\langle s|\hat{H}|s\rangle)^2 = \frac{225}{16}\hbar^2\omega^2$$

$$\Delta H = \sqrt{\langle s|\hat{H}^2|s\rangle - (\langle s|\hat{H}|s\rangle)^2} = \boxed{\sqrt{\frac{67}{16}}\hbar\omega} \sim 2\hbar\omega$$

$$\Delta H = \sqrt{\langle s|\hat{H}^2|s\rangle - (\langle s|\hat{H}|s\rangle)^2} = \boxed{\sqrt{\frac{67}{16}}\, \hbar\omega} \sim 2\hbar\omega$$

d) Compute $\langle m|\hat{x}|n\rangle$ where

$$\hat{x} = i\sqrt{\frac{\hbar}{2m\omega}}\,(\hat{a} - \hat{a}^+) \Rightarrow$$ we need
$\langle m|\hat{a}|n\rangle \propto \delta_{m,n-1}$
$\langle m|a^+|n\rangle \propto \delta_{m,n+1}$

since $\langle m|\hat{x}|n\rangle = A\,\delta_{m,n-1} + B\,\delta_{m,n+1}$

i.e. the only NON-ZERO elements are $m = n \pm 1$

$$\Rightarrow \boxed{\langle S|\hat{x}|S\rangle = 0} \quad \text{AT } \underline{\text{ALL } t}$$

e) $$|S(t)\rangle = e^{-iE_0 t/\hbar}\,\frac{1}{2}|0\rangle + e^{-iE_3 t/\hbar}\,\frac{1}{2}|3\rangle + $$
$$+ e^{-iE_5 t/\hbar}\,\frac{1}{\sqrt{2}}|5\rangle +$$

Let us compute $\langle n|\hat{p}^2|m\rangle$

where $$\hat{p} = \sqrt{\frac{m\hbar\omega}{2}}\,(\hat{a} + \hat{a}^+) = c\,(\hat{a} + \hat{a}^+)$$

$$\hat{p}^2 = c^2(\hat{a}^2 + \hat{a}^{+2} + \hat{a}^+\hat{a} + \hat{a}\hat{a}^+)$$

$$\langle m|\hat{p}^2|n\rangle = c^2\Big\{\sqrt{(n+1)(n+2)}\,\delta_{m,n+2} + \sqrt{n(n-1)}\,\delta_{m,n-2} + $$
$$+ (2n+1)\,\delta_{m,m}\Big\}$$

When computing $\langle S|\hat{p}^2|S\rangle$ the only <u>NON-ZERO</u> elements are

$$\langle 0|\hat{p}^2|0\rangle = c^2$$
$$\langle 3|\hat{p}^2|3\rangle = 7c^2 \qquad \left(c^2 = \frac{m\hbar\omega}{2}\right)$$
$$\langle 5|\hat{p}^2|5\rangle = 11c^2$$

$$\left.\begin{array}{l}\langle 3|\hat{p}^2|5\rangle = \sqrt{20}\,c^2 \\ \langle 5|\hat{p}^2|3\rangle = \sqrt{20}\,c^2\end{array}\right\} \text{ note that } \langle 5|\hat{p}^2|3\rangle^* = \langle 3|\hat{p}^2|5\rangle$$

So, finally, we have

$$\langle S(t)|\hat{p}^2|S(t)\rangle = \frac{1}{4}\langle 0|\hat{p}^2|0\rangle + \frac{1}{4}\langle 3|\hat{p}^2|3\rangle + \frac{1}{2}\langle 5|\hat{p}^2|5\rangle$$
$$+ 2\,\mathrm{Re}\left\{\frac{1}{2\sqrt{2}}e^{i(E_5-E_3)t/\hbar}\langle 5|\hat{p}^2|3\rangle\right\}$$
$$= \frac{m\hbar\omega}{2}\left(\frac{1}{4} + \frac{1}{4}7 + \frac{1}{2}11\right) +$$
$$+ m\hbar\omega\frac{\sqrt{20}}{2\sqrt{2}}\cos(2\omega t) =$$

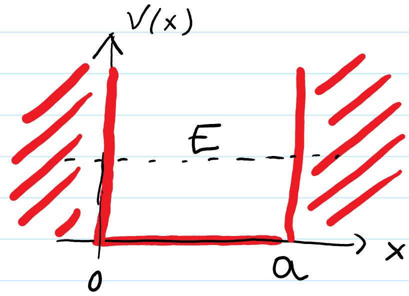
$$[E_5 - E_3 = 2\hbar\omega] \qquad = \boxed{\frac{m\hbar\omega}{2}\left[\frac{15}{2} + \sqrt{10}\cos(2\omega t)\right]}$$

Jan.2021-Pb.2

Monday, January 4, 2021 11:03 AM

Problem #2

a) Textbook derivation:



$$\psi'' = -k^2\psi \qquad k = \sqrt{\frac{2mE}{\hbar^2}}$$

$$\psi(x) = A\sin kx + B\cancel{\cos}\, kx$$

B.C. $\psi(0) = 0 \Rightarrow B = 0$

$\psi(a) = 0 \Rightarrow \sin(ka) = 0$

$$k_n = \frac{n\pi}{a}$$

$$\psi_n(x) = A\sin\left(\frac{n\pi x}{a}\right)$$

normalize $\int_0^a |\psi_n(x)|^2 dx = 1$

$$|A|^2 \int_0^a \sin^2\left(\frac{n\pi x}{a}\right) dx = 1$$

$$|A|^2 \frac{a}{2} = 1 \qquad A = \sqrt{\frac{2}{a}}$$

$$\boxed{\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)}$$

$$k_n^2 = \frac{2mE_n}{\hbar^2}$$

$$\frac{n^2\pi^2}{a^2} = \frac{2mE_n}{\hbar^2}$$

$$\boxed{E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}}$$

b) $\psi(\bar{x}) = \psi_{n_x}(x)\,\psi_{n_y}(y)\,\psi_{n_z}(z)$ { separable problem with factorized solutions }

$$\boxed{\psi(\bar{x}) = \sqrt{\frac{8}{a^3}}\sin\left(\frac{n_x\pi x}{a}\right)\sin\left(\frac{n_y\pi y}{a}\right)\sin\left(\frac{n_z\pi z}{a}\right)}$$

with $\boxed{E_{n_x,n_y,n_z} = (n_x^2 + n_y^2 + n_z^2)\frac{\pi^2\hbar^2}{2ma^2}}$

c) GROUND STATE: $n_x = n_y = n_z = 1$ $\quad E_{111} = \frac{3\pi^2\hbar^2}{2ma^2}$

$$\boxed{\psi_{111} = \sqrt{\frac{8}{a^3}}\sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{\pi y}{a}\right)\sin\left(\frac{\pi z}{a}\right)}$$

$2ma^2$

$$\boxed{\psi_{111} = \sqrt{\frac{8}{a^3}} \sin\left(\frac{\pi x}{a}\right) \sin\left(\frac{\pi y}{a}\right) \sin\left(\frac{\pi z}{a}\right)}$$

no DEGENERACY

FIRST excited state $\begin{pmatrix} n_x = 2 \\ n_y = n_z = 1 \end{pmatrix}$ or $\begin{pmatrix} n_y = 2 \\ n_x = n_z = 1 \end{pmatrix}$ or $\begin{pmatrix} n_z = 2 \\ n_x = n_y = 1 \end{pmatrix}$

$\boxed{3\text{-FOLD}}$ DEGENERATE

$$E_{211} = E_{121} = E_{211} = \boxed{\frac{6\pi^2\hbar^2}{2ma^2}} = \frac{3\pi^2\hbar^2}{ma^2}$$

$$\boxed{\begin{aligned} \psi_{211} &= \sqrt{\frac{8}{a^3}} \sin\left(\frac{2\pi x}{a}\right) \sin\left(\frac{\pi y}{a}\right) \sin\left(\frac{\pi z}{a}\right) \\ \psi_{121} &= \sqrt{\frac{8}{a^3}} \sin\left(\frac{\pi x}{a}\right) \sin\left(\frac{2\pi y}{a}\right) \sin\left(\frac{\pi z}{a}\right) \\ \psi_{112} &= \sqrt{\frac{8}{a^3}} \sin\left(\frac{\pi x}{a}\right) \sin\left(\frac{\pi y}{a}\right) \sin\left(\frac{2\pi z}{a}\right) \end{aligned}}$$

d) "Rules of thumb" $|\langle n|\hat{H}_p|n\rangle| \ll |\langle n|\hat{H}_0|n\rangle|$

$$|\langle k|\hat{H}_p|n\rangle| \ll |E_k^0 - E_n^0|$$

$\Longrightarrow$ in both cases we get (modulo some prefactors of order ~ 1) $\boxed{V_0 \ll \frac{\pi^2\hbar^2}{ma^2}}$

e) For the GROUND STATE, We APPLY NON-DEGENERATE PT

$$E_n^1 = \langle n|\hat{H}_p|n\rangle = \int \psi_n^* V_p \psi_n \, dx$$

$$\boxed{E_{111}^1} = \int_0^a dx \int_0^a dy \int_0^a dz \, |\psi_{111}(xyz)|^2 V_p =$$

$$= \cancel{a^3} V_0 \frac{8}{\cancel{a^3}} \int_0^a dx \sin^2\left(\frac{\pi x}{a}\right) \delta\left(x - \frac{1}{4}a\right) \int_0^a dy \sin^2\left(\frac{\pi y}{a}\right) \delta\left(y - \frac{1}{2}a\right) \times$$

$$\times \int_0^a dz \sin^2\left(\frac{\pi z}{a}\right) \delta\left(z - \frac{3}{4}a\right) =$$

$$= 8 V_0 \underbrace{\sin^2\left(\frac{\pi}{4}\right)}_{1/2} \underbrace{\sin^2\left(\frac{\pi}{2}\right)}_{1} \underbrace{\sin^2\left(\frac{3}{4}\pi\right)}_{1/2} = \boxed{2 V_0}$$

f) FOR THE FIRST EXCITED STATE, we need to use DEGENERATE PT

$\downarrow$

DIAGONALIZE THE MATRIX $\tilde{H}_p$ OF ELEMENTS $\langle i | \hat{H}_p | j \rangle$ in the DEGENERATE SUBSPACE GENERATED BY THE STATES

$$|1\rangle = |n_x = 2, n_y = 1, n_z = 1\rangle$$
$$|2\rangle \equiv |n_x = 1, n_y = 2, n_z = 1\rangle$$
$$|3\rangle \equiv |n_x = 1, n_y = 1, n_z = 2\rangle$$

NOTE THAT ALL ELEMENTS INVOLVING $|2\rangle$ ARE IDENTICALLY ZERO

$$\langle i | \hat{H}_p | 2 \rangle = 0$$

since $\displaystyle\int_0^a dy \sin\left(\frac{n_i \pi y}{a}\right) \sin\left(\frac{2\pi y}{a}\right) \delta\left(y - \frac{a}{2}\right) =$

$$= \sin\left(\frac{n_i \pi}{2}\right) \underbrace{\sin\left(\frac{\cancel{2}\pi}{\cancel{2}}\right)}_{=0!}$$

$$\langle i | H_p | j \rangle \Rightarrow \begin{pmatrix} \langle 1 | H_p | 1 \rangle & 0 & \langle 1 | H_p | 3 \rangle \\ 0 & 0 & 0 \\ \langle 3 | H_p | 1 \rangle & 0 & \langle 3 | H_p | 3 \rangle \end{pmatrix} \equiv \tilde{H}_p$$

$$\langle i|H_p|j\rangle \Rightarrow \begin{pmatrix} \langle 1|H_p|1\rangle & 0 & \langle 1|H_p|3\rangle \\ 0 & 0 & 0 \\ \langle 3|H_p|1\rangle & 0 & \langle 3|H_p|3\rangle \end{pmatrix} \equiv \tilde{H}_p$$

$$\langle 1|H_p|1\rangle = \int_0^a dx \int_0^a dy \int_0^a dz \, |\psi_{211}|^2 V_p = \dots = 4V_0$$

$$\langle 3|H_p|3\rangle = \int_0^a dx \int_0^a dy \int_0^a dz \, |\psi_{112}|^2 V_p = \dots = 4V_0$$

$$\langle 3|H_p|1\rangle = \langle 1|H_p|3\rangle = \int_0^a dx \int_0^a dy \int_0^a dz \, \psi_{112}\psi_{211} V_p = \dots = -4V_0$$

Putting all the values together, we get

$$\tilde{H}_p = V_0 \begin{pmatrix} 4 & 0 & -4 \\ 0 & 0 & 0 \\ -4 & 0 & 4 \end{pmatrix}$$

Let us diagonalize $\tilde{H}_p$. One EIGENVALUE is equal to 0.

$$0 = \det \begin{pmatrix} 4-\lambda & -4 \\ -4 & 4-\lambda \end{pmatrix} = (4-\lambda)^2 - 16 = \lambda^2 - 8\lambda = \underbrace{\lambda(\lambda-8)}$$

which provides the other two eigenvalues being 0, 8

$\Rightarrow$ The FIRST ORDER CORRECTIONS to the first excited state are therefore

$$\boxed{\begin{array}{ll} 0 & \text{2-FOLD DEGENERATE} \\ 8V_0 & \text{NON DEGENERATE} \end{array}}$$

Solutions for Part B

Wednesday, January 6, 2021 12:11 AM

3. (I) $H = \begin{pmatrix} E_1^{(0)} & \lambda V_{12} \\ \lambda V_{21} & E_2^{(0)} \end{pmatrix}$ with $\langle 1^{(0)} | 1^{(0)} \rangle = \langle 2^{(0)} | 2^{(0)} \rangle = 1$, $V_{ij} = \langle i^{(0)} | V | j^{(0)} \rangle$,
and $H^0 | i^{(0)} \rangle = E_i^{(0)} | i^{(0)} \rangle$.

(II) Hermiticity of $H \Rightarrow \begin{cases} \lambda V_{12} = (\lambda V_{21})^* \\ \text{The overall phase of } |1^{(0)}\rangle \text{ (and } |2^{(0)}\rangle\text{) is arbitrary,} \end{cases}$
which can be used to set $\lambda V_{12} = \lambda V_{21} \in R$.

(III) We do not have this freedom if H is non-Hermitian: the inner product is defined differently from quantum mechanics. For the definition mentioned in the problem, it is clear that only the overall sign of $|1^{(0)}\rangle$ (and $|2^{(0)}\rangle$) is arbitrary, which cannot make λV_{12} or λV_{21} real in general.

(IV) $$E_{1,2} = \frac{(E_1^{(0)} + E_2^{(0)})}{2} \pm \sqrt{\frac{(E_1^{(0)} - E_2^{(0)})^2}{4} + |\lambda V_{12}|^2}$$

$$\approx \begin{cases} E_1^{(0)} - \dfrac{|\lambda V_{12}|^2}{E_2^{(0)} - E_1^{(0)}} \\ E_2^{(0)} + \dfrac{|\lambda V_{12}|^2}{E_2^{(0)} - E_1^{(0)}} \end{cases} \qquad (|\lambda V_{12}| \ll |E_1^{(0)} - E_2^{(0)}|)$$

If $E_2^{(0)} > E_1^{(0)}$, then $E_2 > E_2^{(0)} > E_1^{(0)} > E_1$, i.e., $E_{1,2}$ do not cross.

(V) We define $\omega_0 = \dfrac{E_2 - E_1}{\hbar} = \dfrac{E_2^{(0)} - E_1^{(0)}}{\hbar} + 2\dfrac{|\lambda V_{12}|^2}{\hbar(E_2^{(0)} - E_1^{(0)})}$. If the driving freq. $\omega \sim \omega_0$, the student can repeat the derivation of the standard time-dependent perturbation theory to find the probability in $|1^{(0)}\rangle$ at time t is given by

$$\frac{|\lambda V_{12}^{(0)}|^2}{\hbar^2} \frac{\sin^2[(\omega_0 - \omega)t/2]}{(\omega_0 - \omega)^2}$$ to the 1st order with $V(\vec{r}, t) = \lambda V^{(0)}(r) \cos \omega t$.

This maximum is reached at $t = \dfrac{m\pi}{|\omega_0 - \omega|}$ $(m = 1, 3, 5, \cdots)$.

4. (I) $$\langle x | \psi \rangle = \langle x | \frac{1}{E - H_0} V | \psi \rangle + \langle x | \phi \rangle$$

or $\psi(x) = \varphi(x) + \int dx' \underbrace{\langle x | \frac{1}{E - H_0} | x' \rangle}_{\text{Green's function}} \underbrace{\langle x' | V \psi \rangle}_{= V(x')\psi(x') \text{ for a local potential}}$

With the outgoing boundary condition, the Green's function becomes

$$G_+(x, x') \equiv \langle x | \frac{1}{E - H_0 + i\varepsilon} | x' \rangle$$

$$= \int dp' dp \quad \langle x | p' \rangle \langle p' | \frac{1}{E - H_0 + i\varepsilon} | p'' \rangle \langle p'' | x' \rangle$$

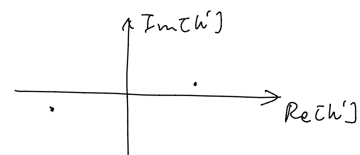
$$= \int dp \quad \frac{e^{+ip'x/\hbar}}{\sqrt{2\pi\hbar}} \quad \frac{1}{E - \frac{p'^2}{2m} + i\varepsilon} \quad \frac{e^{-ip'x'/\hbar}}{\sqrt{2\pi\hbar}}$$

$$= \frac{2m}{2\pi\hbar^2} \int dk' \quad \underbrace{\frac{1}{k^2 - k'^2 + i\tilde{\varepsilon}}}_{\Downarrow} \quad e^{ik'(x-x')}$$

$\left(\begin{array}{l} k' = p'/\hbar \\ \tilde{\varepsilon} = \varepsilon \cdot 2m/\hbar^2 \\ E \equiv (\hbar k)^2/2m \\ (k > 0) \end{array} \right)$

$$\approx \frac{1}{\underbrace{(k + i\tilde{\varepsilon}/2)^2}_{\equiv \tilde{k}} - k'^2} = \left[\frac{1}{k' + \tilde{k}} - \frac{1}{k' - \tilde{k}} \right] \frac{1}{2\tilde{k}}$$

poles at $k' = \pm(k + \tilde{\varepsilon}/2)$



$$\Rightarrow G_+(x, x') = \frac{2m}{2\pi\hbar^2} \begin{cases} (2\pi i)\, e^{ik(x-x')} \left(-\frac{1}{2k}\right) & (x > x') \\ (-2\pi i)\, e^{-ik(x-x')} \left(\frac{1}{2k}\right) & (x < x') \end{cases}$$

$$= -i \frac{m}{\hbar^2 k} e^{ik|x-x'|}$$

$$\Rightarrow \psi(x) = \varphi(x) - i\frac{m}{\hbar^2 k} \int dx' V(x') \psi(x') e^{ik|x-x'|}$$

(II) $\psi(x) = e^{ikx} - i\frac{m}{\hbar^2 k} \int_{-a}^{a} dx' \, V_0 \, \underline{\psi(x')} \, e^{ik|x-x'|}$

1st-order Born approx: $\approx e^{ikx'}$

$$\psi(x) = e^{ikx} - i\frac{m}{\hbar^2 k} V_0 \int_{-a}^{a} dx' \, e^{ikx} \qquad (x > a)$$

$$\Rightarrow \begin{cases} \psi(x) = e^{ikx} - i\frac{m}{\hbar^2 k} V_0 \int_{-a} dx'\, e^{ikx} \qquad (x > a) \\ \quad = e^{ikx}\left[1 - i\frac{mV_0}{\hbar^2 k} 2a\right] = e^{ikx}\left[1 - i\frac{V_0}{E} ka\right] \\ \psi(x) = e^{ikx} - i\frac{m}{\hbar^2 k} V_0 \int_{-a}^{a} dx'\, e^{2ikx'} e^{-ikx} \qquad (x < -a) \end{cases}$$

$$= e^{ikx} - e^{-ikx}\left(i\frac{m}{\hbar^2 k} V_0 \frac{e^{2ika} - e^{-2ika}}{2ik}\right)$$

$$= e^{ikx} - e^{-ikx}\left(i\frac{V_0}{2E}\sin(2ka)\right)$$

(III) So the reflection coeff: $r = -i\frac{V_0}{2E}\sin(2ka)$

and the transmission ~ : $t = 1 - i\frac{V_0}{E} ka$

Clearly, $T = |t|^2 > 1$ which is unsound.

But $R = |r|^2 = \frac{V_0^2}{4E^2}\sin^2(2ka)$ is a good approximation when $|V_0| << E$

The exact result is: $R = 1 - \frac{1}{1 + \frac{V_0^2}{4E}\frac{\sin^2(2ka)}{E - V_0}}$

$$\approx 1 - \frac{1}{1 + \frac{V_0^2}{4E^2}\sin^2(2ka)} \qquad (|V_0| << E)$$

$$\approx \frac{V_0^2}{4E^2}\sin^2(2ka)$$

Qualifying Exam
Quantum Mechanics
June 2021

Problem 1. Consider two observables $\hat{A}$ and $\hat{B}$ in a three-dimensional Hilbert space. In the basis:

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \quad , \quad |2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \quad , \quad |3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} ,$$

the observables $\hat{A}$ and $\hat{B}$ are represented, respectively, by the matrices

$$A \to a \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 6 \end{pmatrix} \quad , \quad B \to b \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 2 \\ 0 & 2 & 0 \end{pmatrix}$$

where $b << a$.

a) [**5 points**] Show that the observables $\hat{A}$ and $\hat{B}$ are not compatible.

Check the commutator $[\hat{A}, \hat{B}]$. Since $\hat{A}$ and $\hat{B}$ do not commute, the observables are NOT compatible. in particular, $\hat{A}$ and $\hat{B}$ do not admit a common set of eigenstates.

b) [**10 points**] Compute the possible outcomes and the corresponding probabilities of separate (independent) measurements of $\hat{A}$ and $\hat{B}$ in the state $|\chi\rangle = \sqrt{\frac{1}{2}}\,(|2\rangle - |3\rangle)$.

$\hat{A}$: in general, we have three possible outcomes in the eigenvalues $a_1 = 1a$, $a_2 = 2a$, $a_3 = 6a$, which correspond to the three eigenstates $|1\rangle$, $|2\rangle$, and $|3\rangle$. The probabilities are given by $P_i = |\langle\chi|i\rangle|^2$, where $i = 1, 2, 3$.

Since $|\chi\rangle = \sqrt{\frac{1}{2}}\,(|2\rangle - |3\rangle)$, we will measure $a_2 = 2a$ with a probability of 50% and $a_3 = 6a$ with a probability of 50%.

$\hat{B}$: the possible outcomes are given by the eigenvalues. Let us firts compute them together with the corresponding eigenstates $|B_1\rangle$, $|B_2\rangle$, and $|B_3\rangle$. The probabilities will be given by $P_i = |\langle\chi|B_i\rangle|^2$, where $i = 1, 2, 3$.

The first eigenvalue is $b_1 = -1b$, and $|B_1\rangle = |1\rangle$. By diagonalizing the sub-matrix $\begin{pmatrix} 0 & 2 \\ 2 & 0 \end{pmatrix}$, we find that the additional eigenvalues are $b_2 = -2b$ and $b_3 = +2b$, with respective eigenvectors $|B_2\rangle = \sqrt{\frac{1}{2}}\,(|2\rangle - |3\rangle)$ and $|B_3\rangle\sqrt{\frac{1}{2}}\,(|2\rangle + |3\rangle)$.

Since $|\chi\rangle = |B_2\rangle$, we will measure $b_2 = -2b$ with a probability of 100%.

c) [**10 points**] Compute the possible outcomes and the corresponding probabilities of a measurements of $\hat{B}$ that follows a measurement of $\hat{A}$, if the system is initially in the state $|\chi\rangle$. What about a measurement of $\hat{A}$ that follows a measurements of $\hat{B}$?

After the measurement of $\hat{A}$, the state of the system will be in $|2\rangle$ or $|3\rangle$ with a probability of 50% each. Noting that $|2\rangle = \sqrt{\frac{1}{2}}\,(|B_2\rangle + |B_3\rangle)$ and $|3\rangle = \sqrt{\frac{1}{2}}\,(|B_2\rangle - |B_3\rangle)$, we can conclude that the measurement of $\hat{B}$ will have a 50% probability of $b_2 = -2b$ a 50% probability of $b_3 = +2b$.

Note that, if we were to perform the measurement of $\hat{B}$ first, it would give a $b_2 = -2b$ with 100% probability and turn the state of the system in — $B_2\rangle$. However, since $|\chi\rangle = |B_2\rangle$, the subsequent measurement of $\hat{A}$ would give the same outcomes as in part b) of the problem.

Let us now construct the Hamiltonian $\hat{H} = \hat{A} + \hat{B}$. Since $b << a$, we can use perturbation theory to study $\hat{H}$.

d) [**10 points**] After writing down the eigenstates and eigenvalues of $\hat{H}_0 = \hat{A}$, compute the first- and second-order corrections to the energy levels due to the correction $\hat{H}_p = \hat{B}$.

Leading Order. (just for defining notation). In the basis defined by

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \quad , \quad |2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \quad , \quad |3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} ,$$

we have $E_1^0 = 1a$, $E_2^0 = 2a$, $E_3^0 = 6a$.
First Order. We use $E_n^1 = \langle n|\hat{H}_p|n\rangle$, to obtain
$E_1^1 = \langle 1|\hat{H}_p|1\rangle = -1b$, $E_2^1 = \langle 2|\hat{H}_p|2\rangle = 0$, $E_3^1 = \langle 3|\hat{H}_p|3\rangle = 0$.
Second Order. Using $E_n^2 = \sum_{k\neq n} \frac{|\langle k|\hat{H}_p|n\rangle|^2}{E_n^0 - E_k^0}$, we get $E_1^2 = 0$, $E_2^2 = -\frac{b^2}{a}$, $E_3^1 = +\frac{b^2}{a}$.
Therefore, up to second order
$E_1 = a - b + \ldots = a\,[1 - X + \mathcal{O}(X^3)]$
$E_2 = 2a - \frac{b^2}{a} + \ldots = a\,[2 - X^2 + \mathcal{O}(X^3)]$
$E_3 = 6a + \frac{b^2}{a} + \ldots = a\,[6 + X^2 + \mathcal{O}(X^3)]$
where $X = b/a$.

e) [**10 points**] Compute the energy eigenstates of $\hat{H}$ up to first order in perturbation theory.

$|p_1^1\rangle = 0$
$|p_2^1\rangle = \sum_{k\neq 2} \frac{\langle k|\hat{H}_p|2\rangle}{E_2^0 - E_k^0}|k\rangle = \frac{\langle 3|\hat{H}_p|2\rangle}{E_2^0 - E_3^0}\;|3\rangle = \frac{2b}{-4a}\;|3\rangle = -\frac{b}{2a}\;|3\rangle$
$|p_3^1\rangle = \sum_{k\neq 3} \frac{\langle k|\hat{H}_p|3\rangle}{E_3^0 - E_k^0}|k\rangle = \frac{\langle 2|\hat{H}_p|3\rangle}{E_3^0 - E_2^0}\;|2\rangle = \frac{2b}{4a}\;|2\rangle = \frac{b}{2a}\;|2\rangle$
Therefore, up to first order:
$|p_1\rangle = |1\rangle$
$|p_2\rangle = |2\rangle - \frac{b}{2a}|3\rangle + \ldots$
$|p_3\rangle = |3\rangle + \frac{b}{2a}|2\rangle + \ldots$

f) [**5 points**] After finding the exact solutions, check that your results for the energy levels obtained in perturbation theory are correct.

By diagonalizing the matrix

$$\hat{H} = a \begin{pmatrix} 1 - X & x & 0 \\ x & 2 & 2X \\ 0 & 2X & 6 \end{pmatrix} ,$$

we get the eigenvalues $\lambda_1 = (1 - X)$ and $\lambda_{2,3} = 4 \mp 2\sqrt{1+x^2}$.
By expanding $\lambda_{2,3}$ for small X, i.e. $\sqrt{1+X^2} = 1 + \frac{1}{2}X^2 + \mathcal{O}(X^4)$, we obtain:
$\lambda_2 = 4 - 2(1 + \frac{1}{2}X^2) = 2 - X^2$,
and
$\lambda_3 = 4 + 2(1 + \frac{1}{2}X^2) = 6 + X^2$,
in agreement with part a).

Time-independent Perturbation Theory:

$$E_n^1 = \langle n|\hat{H}_p|n\rangle; \quad E_n^i = \langle p_n^0|\hat{H}_p|p_n^{i-1}\rangle; \quad |p_n^1\rangle = \sum_{k\neq n} \frac{\langle k|\hat{H}_p|n\rangle}{E_n^0 - E_k^0}|k\rangle$$

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2.a. (10 points) Substituting $\psi_l(r,\theta,\phi) = r^{-1}\chi_l(r)P_l(\cos\theta)$ into

$$-\nabla^2\psi = \frac{2m}{\hbar^2}\left[E - V(r)\right] = \left[k^2 - \frac{2m}{\hbar^2}V(r)\right]\psi,$$

yields

$$-\frac{r}{\chi_l(r)}\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr}\frac{\chi_l(r)}{r} + \frac{l(l+1)}{r^2} = k^2 - \frac{2m}{\hbar^2}V(r),$$

or

$$\frac{d^2\chi_l}{dr^2} + \left[k^2 - \frac{l(l+1)}{r^2} - \frac{2m}{\hbar^2}V(r)\right]\chi_l(r) = 0.$$

Similarly, for the perturbed potential

$$\frac{d^2\chi_l'}{dr^2} + \left\{k^2 - \frac{l(l+1)}{r^2} - \frac{2m}{\hbar^2}\left[V(r) + \delta V(r)\right]\right\}\chi_l'(r) = 0.$$

2.b. (10 points) From the two wave equations above,

$$\chi_l'^{\,*}(r)\frac{d^2\chi_l(r)}{dr^2} - \frac{d^2\chi_l'^{\,*}(r)}{dr^2}\chi_l(r) = -\frac{2m}{\hbar^2}\delta V(r)\ \chi_l'^{\,*}(r)\chi_l(r).$$

The left-hand side is the derivative with respect to r of

$$\chi_l'^{\,*}(r)\frac{d\chi_l(r)}{dr} - \frac{d\chi_l'^{\,*}(r)}{dr}\chi_l(r) \approx k\sin\left(kr - \frac{\pi l}{2} + \delta_l'\right)\cos\left(kr - \frac{\pi l}{2} + \delta_l\right)$$
$$-k\cos\left(kr - \frac{\pi l}{2} + \delta_l'\right)\sin\left(kr - \frac{\pi l}{2} + \delta_l\right) = k\sin(\delta_l' - \delta_l),$$

for large r. Thus

$$\sin(\delta_l' - \delta_l) = \frac{1}{k}\int_0^\infty\left[\chi_l'^{\,*}(r)\frac{d^2\chi_l(r)}{dr^2} - \frac{d^2\chi_l'^{\,*}(r)}{dr^2}\chi_l(r)\right] = -\frac{2m}{\hbar^2 k}\int_0^\infty \delta V(r)\ \chi_l'^{\,*}(r)\chi_l(r)dr.$$

2.c. (10 points) For $\delta_l' - \delta_l$ small, we can drop the sine in the expression above, yielding

$$\delta_l' = \delta_l - \frac{2m}{\hbar^2 k}\int_0^\infty \delta V(r)\ |\chi_l(r)|^2 dr,$$

where we have replaced $\chi_l'(r)$ by $\chi_l(r)$.

2.d. (10 points) We replace δ_l by zero, δ_l' by δ_l and $\chi_l(r)$ by the solution with $f(\theta) = 0$, namely $i^l j_l(kr)$. Thus

$$\delta_l = -\frac{2m}{\hbar^2 k} \int_0^\infty V(r)\ j_l(kr)^2 dr.$$

Changing the sign of the potential changes the sign of the all of the phase shifts.

2.e. (10 points) If r_0 is sufficiently small, then the integrand is small except where

$$j_l(kr) \approx \frac{2^l l!}{(2l+1)!} k^l r^l.$$

Thus

$$\delta_l \approx -\frac{2^{2l+1}(l!)^2}{[(2l+1)!]^2} \frac{mV_0 k^{2l-1}}{\hbar^2} \int_0^\infty r^{2l} e^{-2r^2/r_0^2} dr.$$

Substituting $u = 2r^2/r_0^2$, $r = \frac{r_0}{2^{1/2}} u^{1/2}$, this becomes

$$\delta_l \approx -\frac{2^{2l+1}(l!)^2}{[(2l+1)!]^2} \frac{mV_0 k^{2l-1}}{\hbar^2} \frac{r_0^{2l+1}}{2^{l+1/2}} \int_0^\infty du\, u^l e^{-u} = -\frac{2^{l+1/2}(l!)^3}{[(2l+1)!]^2} \frac{mV_0 k^{2l-1} r_0^{2l+1}}{\hbar^2},$$

where we have used

$$\int_0^\infty du\, u^l e^{-u} = \Gamma(l+1) = l!.$$

Some useful definitions and formulas:

Legendre polynomials $P_l(z)$:

$$(1-z^2)\frac{d^2}{dz^2}P_l(x) - 2z\frac{dP_l(z)}{dz} + l(l+1)P_l(z) = 0, \ \int_{-1}^{1} P_k(z)P_l(z)\,dz = \frac{2\delta_{kl}}{2l+1},$$

$$P_0(z) = 1, \ P_1(z) = z, \ P_2(z) = \frac{1}{2}(3z^2 - 1), \ P_3(z) = \frac{1}{2}(5z^3 - 1), \ \dots .$$

Spherical Bessel functions $j_l(\rho)$:

$$e^{\mathrm{i}\rho z} = \sum_{l=0}^{\infty}(2l+1)\mathrm{i}^l j_l(\rho)P_l(z),$$

$$\frac{1}{\rho^2}\frac{d}{d\rho}\left[\rho^2\frac{dj_l(\rho)}{d\rho}\right] + \left[1 - \frac{l(l+1)}{\rho^2}\right] j_l(\rho) = 0,$$

$$j_l(\rho) = (-\rho)^l\left(\frac{1}{\rho}\frac{d}{d\rho}\right)^l \frac{\sin\rho}{\rho} \longrightarrow \frac{2^l l!}{(2l+1)!}\rho^l, \text{ as } \rho \to 0,$$

$$j_l(\rho) \longrightarrow \frac{1}{\rho}\cos\left(\rho - \frac{\pi l}{2}\right), \text{ as } \rho \to \infty.$$

The partial wave expansion for positive-energy eigenfunctions. with $\vec{k} = k\hat{z}$:

$$\psi_k(r,\theta) \longrightarrow e^{\mathrm{i}kr\cos\theta} + \frac{f(\theta)}{r}e^{\mathrm{i}kr}, \text{ as } r \to \infty,$$

$$f(\theta) = \frac{1}{2\mathrm{i}k}\sum_{l=0}^{\infty}(2l+1)(e^{2\mathrm{i}\delta_l} - 1)P_l(\cos\theta).$$

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Solutions

Problem 1.
Consider a spin-1 particle in the state:

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

where $|+\rangle \equiv |s=1, s_z=1\rangle$, $|0\rangle \equiv |s=1, s_z=0\rangle$, and $|-\rangle \equiv |s=1, s_z=-1\rangle$ are the eigenstates of $\hat{S}_z$.

1.a) (5 points) Show that the $\hat{S}_z$ operator can be written as $\hat{S}_z = \hbar(|+\rangle\langle+|) - \hbar(|-\rangle\langle-|)$. Write the expression for the operator $\hat{S}_z^2$.

Textbook problem. The simplest way is to use the spectral decomposition $\hat{A} = \sum_i |a_i\rangle\lambda_i\langle a_i|$, where $|a_i\rangle$ and λ_i are the eigenvectors and eigenvalues of the operator $\hat{A}$, respectively.
By squaring $\hat{S}_z$, we obtain $\hat{S}_z^2 = \hbar^2|+\rangle\langle+| + |-\rangle\langle-|$.
In matrix form (if need be) this would be represented by

$$\hat{S}_z \to \hbar\begin{pmatrix}1 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & -1\end{pmatrix} \quad , \quad \hat{S}_z^2 \to \hbar^2\begin{pmatrix}1 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & 1\end{pmatrix}.$$

1.b) (15 points) Beginning with the state $|\psi\rangle$, consider measuring first $\hat{S}_z^2$, then measuring afterwards $\hat{S}_z$. What are the possible measurement outcomes of $\hat{S}_z^2$ and the corresponding probabilities? What are the possible outcomes of a measurement of $\hat{S}_z$ after $\hat{S}_z^2$ has been measured and the corresponding probabilities?

First measurement ($\hat{S}_z^2$): The possible outcomes are given by the eigenvalues of $\hat{S}_z^2$, which are 0 (non degenerate) and $\hbar^2$ (degenerate of degree 2) respectively. We will measure $S_z^2 = 0$ with probability $P_0 = |\langle\psi|0\rangle|^2 = \frac{1}{3}$. We will measure $S_z^2 = \hbar^2$ with probability $P_+ = |\langle\psi|1\rangle|^2 = \frac{2}{3}$, where $|1\rangle = \sqrt{\frac{1}{2}}\Big(|+\rangle + |-\rangle\Big)$ is the eigenstate of eigenvalue $\hbar^2$ and the state of the system after the measurement. Note that the from of $|1\rangle$ can be obtained directly (by observing the form of the operator S_z^2 and the initial state of the system) or by applying the projector $P = |+\rangle\langle+| + |-\rangle\langle-|$ to the initial state of the system and normalizing the outcome.
Second measurement ($\hat{S}_z$): If the outcome of the first measurement was $S_z^2 = 0$, the system is now in the state $|0>$. We will then measure $S_z = 0$ with probability $P_0 = |\langle 0|0\rangle|^2 = 1$.
If the outcome of the first measurement was $S_z^2 = 1$, the system is now in the state $|1\rangle = \sqrt{\frac{1}{2}}\Big(|+\rangle + |-\rangle\Big)$. We will then measure $S_z = \hbar$ with probability $P_+ = |\langle 1|+\rangle|^2 = \frac{1}{2}$ and $S_z = -\hbar$ with probability $P_- = |\langle 1|-\rangle|^2 = \frac{1}{2}$.

Assume the Hamiltonian of the system to be

$$\hat{H} = A\hat{S}_z^2 + B(\hat{S}_x^2 - \hat{S}_y^2).$$

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1.a. (10 points) The time derivatives of the components of the position vector are

$$\frac{dr^j}{dt} = \frac{1}{\mathrm{i}\hbar}[H, r^j] = \frac{1}{\mathrm{i}\hbar}[-\mathrm{i}\hbar c\vec{\alpha}\cdot\vec{\nabla}, r^j] = -c\alpha_j,$$

or

$$\frac{d\vec{r}}{dt} = -c\vec{\alpha}.$$

(Note: this illustrates the phenomenon of *Zitterbewegung*, which is that the expectation value of the velocity of the massive electron has magnitude c. The electron's path fluctuates, resulting in an average velocity $< c$.) The time derivatives of the components of the momentum vector are

$$\frac{dp_j}{dt} = \frac{1}{\mathrm{i}\hbar}[H, p_j] = \frac{1}{\mathrm{i}\hbar}\left[-ec\vec{\alpha}\cdot\vec{A}(\vec{r},t) + e\phi(\vec{r},t)\ ,\ -\mathrm{i}\hbar\frac{\partial}{\partial r^j}\right] = -ec\frac{\partial}{\partial r^j}\left(\vec{\alpha}\cdot\vec{A}\right) + e\frac{\partial\phi}{\partial r^j},$$

so the velocity operator is

$$\frac{d\vec{p}}{dt} = -ec\vec{\nabla}\left(\vec{\alpha}\cdot\vec{A}\right) + e\vec{\nabla}\phi.$$

1.b. (10 points) The time derivative of $\vec{p} - e\vec{A} = m\vec{v}$ (the force on the electron) is

$$\vec{F} = \frac{d}{dt}(\vec{p} - e\vec{A}) = \frac{d\vec{p}}{dt} - e\left(\frac{1}{\mathrm{i}\hbar}[H,\vec{A}] + \frac{\partial\vec{A}}{\partial t}\right) = -ec\vec{\nabla}(\vec{\alpha}\cdot\vec{A}) + e\vec{\nabla}\phi + ec(\alpha\cdot\vec{\nabla})\vec{A} - e\frac{\partial\vec{A}}{\partial t}.$$

(Had you found this time derivative of $\vec{p} - e\vec{A}$ above, you would have received full credit for Part b., but we remark that using the formulas for the electric and magnetic fields respectively,

$$\vec{E} = -\vec{\nabla}\phi + \frac{\partial\vec{A}}{\partial t},\ \ \vec{B} = \vec{\nabla}\times\vec{A},$$

it may be written as

$$\vec{F} = -e(\vec{E} + c\vec{\alpha}\times\vec{B}),$$

the Lorentz force of a particle with velocity $\vec{v} = c\vec{\alpha}$.)

We now have

$$\frac{d\vec{L}}{dt} = \frac{d\vec{r}}{dt}\times(\vec{p} - e\vec{A}) + \vec{r}\times\frac{d}{dt}(\vec{p} - e\vec{A}) = -c\vec{\alpha}\times(\vec{p} - e\vec{A}) + \vec{r}\times\vec{F},$$

where $\vec{F}$ is the force given above.

1.c. (10 points) From Part a., we have

$$\vec{\tau} = \vec{r} \times \vec{F}.$$

It is acceptable to write this as either of the two expressions

$$\vec{\tau} = -e\vec{r} \times \left[-\vec{\nabla}\phi + \frac{\partial \vec{A}}{\partial t} + c\vec{\nabla}(\vec{\alpha} \cdot \vec{A}) - c(\vec{\alpha} \cdot \vec{\nabla})\vec{A} \right] = -\vec{r} \times e \left(\vec{E} + c\vec{\alpha} \times \vec{B} \right).$$

1.d. (20 points) We have that β commutes with S^j, $j = x, y, z$, so that (again implicitly summing over repeated indices)

$$\frac{dS^j}{dt} = \frac{1}{\mathrm{i}\hbar}[H, S^j] = -\frac{\mathrm{i}c}{2}(p_k - eA_k) \left[\begin{pmatrix} \sigma_k & 0 \\ 0 & -\sigma_k \end{pmatrix}, \begin{pmatrix} \sigma_j & 0 \\ 0 & \sigma_j \end{pmatrix} \right],$$

where the index k is summed implicitly. This simplifies to

$$\frac{dS^j}{dt} = -\frac{\mathrm{i}c}{2}(p_k - eA_k) 2\mathrm{i}\varepsilon^{kjl} \begin{pmatrix} \sigma_l & 0 \\ 0 & -\sigma_l \end{pmatrix} = c\varepsilon^{kjl}(p_k - eA_k)\alpha^l,$$

or

$$\frac{d\vec{S}}{dt} = -c(\vec{p} - e\vec{A}) \times \vec{\alpha} = c\vec{\alpha} \times (\vec{p} - e\vec{A}).$$

The time derivative of the total angular momentum $\vec{J} = \vec{L} + \vec{S}$, is from this result and from Part b.,

$$\frac{d\vec{J}}{dt} = -c\vec{\alpha} \times (\vec{p} - e\vec{A}) + \vec{r} \times \vec{F} + c\vec{\alpha} \times (\vec{p} - e\vec{A}) = \vec{r} \times \vec{F} = \vec{\tau},$$

i.e., the torque.

1.c) (5 points) Show that, in the basis of eigenstates of $\hat{S}_z$, the operators $\hat{S}_x$ and $\hat{S}_y$ have the form:

$$\hat{S}_x \to \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \quad , \quad \hat{S}_y \to \frac{i\hbar}{\sqrt{2}}\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} .$$

Textbook calculation. One common way is to use the operators S_+ and S_-, given in the formulae, and then build the linear combinations using $S_\pm = S_x \pm iS_y$.

1.d) (10 points) Find the matrix representation of $\hat{H}$, in the basis of eigenstates of $\hat{S}_z$.

Using the expressions of S_x, S_y, and S_z, which were given in 1.c) and 1.a), one can easily obtain

$$\hat{H} \to \hbar^2 \begin{pmatrix} A & 0 & B \\ 0 & 0 & 0 \\ B & 0 & A \end{pmatrix} .$$

1.e) (10 points) Solve the problem exactly, to find the eigenvalues and eigenstates of $\hat{H}$.

The energy eigenstates and eigenvalues are: $|E_\pm\rangle = \sqrt{\frac{1}{2}}\Big(|+\rangle \pm |-\rangle\Big)$ with eigenvalues $E_\pm = \hbar^2(A \pm B)$ and $|E_0\rangle = |0\rangle$ with eigenvalue $E_0 = 0$.

1.f) (5 points) Compute the expectation value of the energy in the state $|\psi\rangle$.

Compute $\langle \hat{H} \rangle_\psi = \langle \psi | \hat{H} | \psi \rangle = \sum_i E_i |\langle \psi | E_i \rangle|^2$ to obtain $\langle \hat{H} \rangle_\psi = \frac{2}{3}\hbar^2(A + B)$.

Qualifying Exam
Quantum Mechanics
June 2022

Solutions

Problem 1.
Let's consider a perturbation H_p to a one-dimensional harmonic oscillator. The Hamiltonian of the system can be written as

$$\hat{H} = \hat{H}_0 + \hat{H}_p \quad \text{where} \quad \hat{\mathrm{H}}_0 = \frac{\hat{\mathrm{p}}^2}{2\mathrm{m}} + \frac{1}{2}\mathrm{m}\omega^2\hat{\mathrm{x}}^2 \quad \text{and} \quad \hat{\mathrm{H}}_\mathrm{p} = \beta\hat{\mathrm{x}}^4$$

Define the operators $\hat{a}$ and $\hat{a}^\dagger$ as

$$\hat{a} = \frac{1}{\sqrt{2m\omega\hbar}}\left(\hat{p} - im\omega\hat{x}\right) \qquad \hat{a}^\dagger = \frac{1}{\sqrt{2m\omega\hbar}}\left(\hat{p} + im\omega\hat{x}\right)$$

1.a) Using the properties of the ladder operators $\hat{a}$ and $\hat{a}^\dagger$, find the expression for all the non-vanishing matrix elements $\langle m|\hat{x}^2|n\rangle$, where $|n\rangle$ and $|m\rangle$ are eigenstates of the unperturbed Hamiltonian $\hat{H}_0$ [15 points].

We should evaluate all non-zero matrix elements $\langle m|\hat{x}^2|n\rangle$, namely the cases $m = -2, 0, +2$. All other matrix elements are zero.
Since $\hat{x} = i\sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a}^\dagger - \hat{a}\right)$, then $\hat{x}^2 = -\frac{\hbar}{2m\omega}\left(\hat{a}^\dagger - \hat{a}\right)\left(\hat{a}^\dagger - \hat{a}\right)$.
Using $\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$ and $\hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$, we get:
$\langle n|\hat{x}^2|n\rangle = \frac{\hbar}{2m\omega}(2n+1)$
$\langle n|\hat{x}^2|n-2\rangle = -\frac{\hbar}{2m\omega}\sqrt{n(n-1)}$
$\langle n|\hat{x}^2|n+2\rangle = -\frac{\hbar}{2m\omega}\sqrt{(n+2)(n+1)}$

1.b) Evaluate the expectation value $\langle n|\hat{x}^4|n\rangle$ [15 points]. *Hint: You can simplify this calculation by using the completeness relation for the energy eigenstates and the result of part 1.a.*

We can compute directly $\langle n|\hat{x}^4|n\rangle$, starting from the expression $\hat{x}^4 = \frac{\hbar^2}{4m^2\omega^2}\left(\hat{a}^\dagger - \hat{a}\right)^4$ or use the hint provided in the text. We will follow the latter route.
Using completeness, we can write: $\langle n|\hat{x}^4|n\rangle = \sum_m \langle n|\hat{x}^2|m\rangle\langle m|\hat{x}^2|n\rangle = \sum_m \left|\langle n|\hat{x}^2|m\rangle\right|^2$ Using the expressions from part 1.b, we finally get:
$\langle n|\hat{x}^4|n\rangle = \frac{\hbar^2}{4m^2\omega^2}\left[(2n+1)^2 + n(n-1) + (n+1)(n+2)\right] = \frac{\hbar^2}{4m^2\omega^2}\left[(6n^2 + 6n + 3\right]$.

1.c) Write the energy spectrum for the Hamiltonian $\hat{H}$ up to first order in perturbation theory [10 points].

The spectrum E_n will be given by $E_n = E_n^0 + E_n^1 + \ldots$ where $E_n^0 = \hbar\omega\left(n + \frac{1}{2}\right)$ (Harmonic oscillator) and $E_n^1 = \langle n|\hat{H}_p|n\rangle = \beta\langle n|\hat{x}^4|n\rangle = \frac{\beta\hbar^2}{4m^2\omega^2}\left[(6n^2 + 6n + 3\right]$.
Thus, $E_n = \hbar\omega\left(n + \frac{1}{2}\right) + \frac{\beta\hbar^2}{4m^2\omega^2}\left[(6n^2 + 6n + 3\right] + \ldots$

1.d) (5 points) Evaluate the commutator $[\hat{H}_0, \hat{H}_p]$.

The evaluation the commutator $[\hat{H}_0, \hat{H}_p]$ comes down to the evaluation of $[\hat{p}^2, \hat{x}^4] = -4ih(\hat{p}\hat{x}^3 + \hat{x}^3\hat{p})$.

1.e) (5 points) Given the result for the commutator in part 1.d), should we expect higher-order corrections to the energy spectrum of H? (Explain your reasoning).

Since their $[\hat{p}^2, \hat{x}^4]$ is not equal to zero, we do not have a complete basis in which the two operators $\hat{H}_0$ and $\hat{H}_p$ are diagonal at the same time.
In particular, the basis of eigenstates of $\hat{H}_0$ is not a basis of eigenstates for the perturbation $\hat{H}_p$ (or the full Hamiltonian $\hat{H}$. As a consequences, we can expect higher order corrections to the energy levels, which should be computed in perturbation theory.

Some useful definitions and formulas:

One-dimensional Harmonic oscillator:

$$\hat{H}_0 = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2, \quad \hat{a} = \frac{1}{\sqrt{2m\omega\hbar}}\,(\hat{p} - im\omega\hat{x}), \quad \hat{a}^\dagger = \frac{1}{\sqrt{2m\omega\hbar}}\,(\hat{p} + im\omega\hat{x}),$$

$$[\hat{a}, \hat{a}^\dagger] = 1, \quad [\hat{H}_0, \hat{a}^\dagger] = \hbar\omega\hat{a}^\dagger,$$

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle, \quad \hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$$

Time-independent Perturbation Theory:

$$E_n^1 = \langle n|\hat{H}_p|n\rangle, \quad E_n^i = \langle p_n^0|\hat{H}_p|p_n^{i-1}\rangle, \quad |p_n^1\rangle = \sum_{k\neq n} \frac{\langle k|\hat{H}_p|n\rangle}{E_n^0 - E_k^0}|k\rangle, \quad E_n^2 = \sum_{k\neq n} \frac{|\langle k|\hat{H}_p|n\rangle|^2}{E_n^0 - E_k^0}\,.$$

Qualifying Exam Solutions, Quantum Mechanics, June 8, 2022

2. Consider the attractive central potential $V(\vec{r}) = -\Omega/r^2$ for a particle of mass m, with $\Omega > 0$.

2.a. (20 points) Write the differential equation for $\chi_l(r) = R_l(r)r$, where R_l is the radial part of the eigenfunction (see the mathematical formulas below). This equation should only contain the radial variable r, not the angular variables θ, ϕ. Note that $R_l(r)$ must be finite at the origin $r = 0$, which gives a boundary condition on $\chi_l(r)$ at $r = 0$. Furthermore, $R_l(r)$ may depend on additional quantum numbers (which are not essential to know for this exercise).

Solution: The spherical harmonic $Y_{lm}(\theta,\phi)$ is an eigenfunction of $\vec{L}^2$ with eigenvalue $\hbar^2 l(l+1)$. Multiplying the eigenvalue equation by $2m/\hbar^2$, after substituting $\hbar^2 l(l+1)$ for $\vec{L}^2$, we find $\chi_l(r)$ satisfies the radial equation

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

For the central potential $u(r) = -L(L+1)/r^2$, the radial equation is

$$\frac{d^2\chi_l(r)}{dr^2} + \left[\varepsilon + \frac{L(L+1) - l(l+1)}{r^2}\right]\chi_l(r) = 0,$$

2.b. (10 points) Next consider the scattering problem. Show that for the special value $\Omega = \frac{\hbar^2 L(L+1)}{2m}$, L being a positive integer, the phase shift of the $l = L$ partial wave, is $\delta_L = L\pi/2$. Do not forget the boundary condition at $r = 0$.

Solution: Recall that

$$\psi(r,\theta) = \sum_{l=0}^{\infty} \frac{(2l+1)\mathrm{i}^l}{r}\chi_l(r)P_l(\cos\theta),$$

where $\chi_l(r)$ satisfies the radial equation with $\varepsilon = k^2$.

$$\frac{d^2\chi_l(r)}{dr^2} + \left[k^2 + \frac{L(L+1) - l(l+1)}{r^2}\right]\chi_l(r) = 0,$$

with $u(r) = 2mV(r)/\hbar^2$. For $l = L$, we have $\frac{d^2\chi_L(r)}{dr^2} + k^2\chi_L(r) = 0$. This must satisfy the boundary condition that $\chi_L(0) = 0$. Thus $\chi_L(r) = A_L \sin kr = A_L \sin(kr - \frac{L\pi}{2} + \delta_L)$ and $\delta_L = L\pi/2$ (not zero, except for $L = 0$).

2.c. (10 points) If $\Omega = \frac{\hbar^2}{m}$, what is the approximate form for the scattering amplitude $f(\theta)$, in terms of δ_0? Include only the contribution from the first two phase shifts, δ_0 and δ_1. You do not have to find δ_0.

This is the $L = 1$ case. For $\Omega = \frac{\hbar^2}{m} = \frac{\hbar^2}{2m} \cdot 1(1+1)$, we have $\delta_1 = \pi/2$. Thus $e^{2i\delta_1} = -1$. Ignoring partial waves beyond $l = 1$, we have

$$f(\theta) \approx \frac{1}{2ik} \sum_{l=0}^{1} (2l+1)(e^{2i\delta_l} - 1) P_l(\cos\theta) = \frac{e^{2i\delta_0} - 1 - 6\cos\theta}{2ik}.$$

2.d. (10 points) Find the Born approximation for $f(\theta)$ for $\Omega = \frac{\hbar^2}{m}$.

Solution: The Born approximation for $f(\theta)$, with $u(r) = -\Omega/r^2$ is

$$f(\theta) = -\frac{1}{4\pi} \int d^3r \, e^{-i(\vec{k}' - \vec{k})\cdot\vec{r}} u(\vec{r}) = \frac{m\Omega}{2\pi\hbar^2} \int \frac{d^3r}{r^2} \, e^{-i(\vec{k}' - \vec{k})\cdot\vec{r}},$$

where $(\vec{k}' - \vec{k})^2 = 2k^2 - 2k^2\cos\theta = 4k^2 \sin^2\frac{\theta}{2}$. Now

$$\int d^3r \, e^{-ik\cdot r} \frac{1}{r^2} = \frac{2\pi^2}{k}.$$

Thus

$$f(\theta) = \frac{m\Omega}{2\pi\hbar^2} \frac{2\pi^2}{|\vec{k}' - \vec{k}|} = \frac{\pi\Omega m}{2\hbar^2 k |\sin\frac{\theta}{2}|} = \frac{\pi\Omega m}{2\hbar^2 k \sin\frac{\theta}{2}}.$$

For $\Omega = \hbar^2/m$, this is

$$f(\theta) = \frac{\pi}{2k\sin\frac{\theta}{2}}.$$

One drawback of the Born approximation is that it is purely real, so does not agree well with the result of Part c.