PHY 742 Spring 2025 Solutions to First Exam

The value of each question is listed in square brackets at the start of the problem or part.

1. [15] A spin-½ particle has state operator $\rho = \begin{pmatrix} a & b \\ b & a \end{pmatrix}$**. You will also need** $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$**.**

(a) [6] What are the eigenvalues of this state operator? What restrictions on *a* and *b* are necessary for it to be a valid state operator? For what value(s) is it a pure state?

The eigenvalues can be determined using the characteristic equation; that is,

$$0 = \det\left(\rho - \lambda \mathbf{1}\right) = \det\begin{pmatrix} a-\lambda & b \\ b & a-\lambda \end{pmatrix} = \left(a-\lambda\right)^2 - b^2 ,$$

$$a - \lambda = \pm b ,$$

$$\lambda = a \pm b$$

To make a valid state operator, the sum of the eigenvalues must be 1, so $1 = a + b + a - b$, or $a = \frac{1}{2}$. The eigenvalues also have to be non-negative, which implies $a \pm b \ge 0$, so $|b| \le a = \frac{1}{2}$. A pure state has only eigenvalues of 1 and 0, which happens if $b = \pm\frac{1}{2}$.

(b) [4] If we measured $S_x = \frac{1}{2}\hbar\sigma_x$**, what would be the expectation value?**

The expectation value of an operator is given by

$$\langle S_x \rangle = \mathrm{Tr}\left(\rho S_x\right) = \frac{\hbar}{2}\mathrm{Tr}\left[\begin{pmatrix} a & b \\ b & a \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\right] = \frac{\hbar}{2}\mathrm{Tr}\begin{pmatrix} b & a \\ a & b \end{pmatrix} = \frac{\hbar}{2}(2b) = b\hbar .$$

(c) [5] If the Hamiltonian is $H = \omega S_x$**, for what values would** ρ **be time-independent?**

We use the equation

$$i\hbar\frac{d}{dt}\rho = \left[H, \rho\right] = \frac{\hbar}{2}\omega\left[\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} a & b \\ b & a \end{pmatrix}\right] = \frac{\hbar}{2}\omega\left\{\begin{pmatrix} b & a \\ a & b \end{pmatrix} - \begin{pmatrix} b & a \\ a & b \end{pmatrix}\right\} = 0.$$

It follows that it is always time-independent.

2. **[15] This problem should be worked entirely in terms of the Heisenberg formulation. A particle is described exclusively in terms of its spin. The Hamiltonian is given by** $H = \omega S_z$.

(a) **[5] Find in this formalism equations for all three time derivatives** $\frac{d}{dt} S_i(t)$.

We use the formula for the derivative of an operator in this formalism,

$$\frac{d}{dt} S_x = \frac{i}{\hbar}\omega[S_z, S_x] = \frac{i}{\hbar}\omega i\hbar S_y = -\omega S_y ,$$
$$\frac{d}{dt} S_y = \frac{i}{\hbar}\omega\left[S_z, S_y\right] = \frac{i}{\hbar}\omega\left(-i\hbar S_x\right) = \omega S_x ,$$
$$\frac{d}{dt} S_z = \frac{i}{\hbar}A[S_z, S_z] = 0 .$$

(b) **[2] Argue that one of the three is time independent, *i.e.*** $S_C(t) = S_C(0)$.

Obviously, since S_z has no time derivative, it is constant, so $S_z(t) = S_z(0)$.

(c) **[8] Check that the other two differential equations can be satisfied by the equations** $S_A(t) = \cos(\omega t) S_A(0) + \sin(\omega t) S_B(0)$ **and** $S_B(t) = \cos(\omega t) S_B(0) - \sin(\omega t) S_A(0)$.

We will make a guess that A is y and B is x. Taking time derivatives, we then have

$$\frac{d}{dt} S_y(t) = \frac{d}{dt}\left[\cos(\omega t) S_y(0) + \sin(\omega t) S_x(0)\right] = \omega\left[-\sin(\omega t) S_y(0) + \cos(\omega t) S_x(0)\right] = \omega S_x(t),$$
$$\frac{d}{dt} S_x(t) = \frac{d}{dt}\left[\cos(\omega t) S_x(0) - \sin(\omega t) S_y(0)\right] = \omega\left[-\sin(\omega t) S_x(0) - \cos(\omega t) S_y(0)\right] = -\omega S_y(t).$$

Obviously, these equations match the previous ones. Had we guessed wrong, it would have failed, basically because we would need to replace ω by $-\omega$.

3. [15] A particle of mass *m* in one dimension is in the potential $V(x)=\begin{cases}\frac{1}{2}m\omega_1^2x^2 & x<0,\\ \frac{1}{2}m\omega_2^2x^2 & x>0.\end{cases}$

Using the WKB method, estimate the energy of the *n*'th eigenstate.

We first need to find the turning points, the points where $V(x)=E$. For $x < 0$, this would be when $\frac{1}{2}m\omega_1^2a^2=E$, or $a=-\frac{1}{\omega_1}\sqrt{\frac{2E}{m}}$, and similarly for $x > 0$, $b=\frac{1}{\omega_2}\sqrt{\frac{2E}{m}}$. We then set up the integral for the WKB approximation and use the possibly helpful integrals to figure it out. For $x < 0$, we will change $x \rightarrow -x$ to make the integrals look a little better.

$$\begin{aligned}
\pi\hbar\left(n+\tfrac{1}{2}\right) &= \int_a^b \sqrt{2m\left[E-V(x)\right]}dx \\
&= \int_{-\sqrt{2E/m}/\omega_1}^{0} \sqrt{2m\left[E-\tfrac{1}{2}m\omega_1^2x^2\right]}dx + \int_0^{\sqrt{2E/m}/\omega_2} \sqrt{2m\left[E-\tfrac{1}{2}m\omega_2^2x^2\right]}dx \\
&= \int_0^{\sqrt{2E/m}/\omega_1} \sqrt{2mE-m^2\omega_1^2x^2}\,dx + \int_0^{\sqrt{2E/m}/\omega_2} \sqrt{2mE-m^2\omega_2^2x^2}\,dx \\
&= \frac{1}{2}\left[\frac{2mE}{m\omega_1}\sin^{-1}\left(\frac{xB}{\sqrt{A}}\right)+x\sqrt{2mE-m^2\omega_1^2x^2}\right]_0^{\sqrt{2E/m}/\omega_1} \\
&\quad +\frac{1}{2}\left[\frac{2mE}{m\omega_2}\sin^{-1}\left(\frac{xB}{\sqrt{A}}\right)+x\sqrt{2mE-m^2\omega_2^2x^2}\right]_0^{\sqrt{2E/m}/\omega_2} \\
&= \frac{E}{\omega_1}\sin^{-1}(1)+\frac{E}{\omega_2}\sin^{-1}(1)=\frac{\pi E}{2}\left(\frac{1}{\omega_1}+\frac{1}{\omega_2}\right).
\end{aligned}$$

Solving for the energy, we have

$$E=\frac{\hbar(2n+1)}{\frac{1}{\omega_1}+\frac{1}{\omega_2}}=\frac{\hbar(2n+1)\omega_1\omega_2}{\omega_1+\omega_2}.$$

4. [15] A particle of mass *m* in one dimension is in the potential $V(x) = B|x|$. Estimate the ground state energy by the variational method using the trial wave function $\psi(x) = e^{-Ax^2/2}$.

The variational method always yields an upper bound on the ground state. For the first excited state because the potential is symmetric, we expect the first excited state to be anti-symmetric, and since our trial wave function is anti-symmetric, it will also be an upper bound on the energy of the first excited state.

In each case, we first compute $\langle\psi|\psi\rangle$, $\langle P^2\rangle$, and $\langle V\rangle$. For the first case, we have

$$\langle\psi|\psi\rangle = \int_{-\infty}^{\infty} |\psi|^2\, dx = \int_{-\infty}^{\infty} e^{-Ax^2}\, dx = 2\int_0^{\infty} e^{-Ax^2}\, dx = \frac{2\Gamma\left(\frac{1}{2}\right)}{2A^{1/2}} = \sqrt{\frac{\pi}{A}},$$

$$\langle P^2\rangle = \left\|P|\psi\rangle\right\|^2 = \int_{-\infty}^{\infty} \left|-i\hbar\frac{\partial\psi}{\partial x}\right|^2 dx = \hbar^2\int_{-\infty}^{\infty} \left|-Axe^{-Ax^2/2}\right|^2 dx = 2\hbar^2 A^2\int_0^{\infty} x^2 e^{-Ax^2}\, dx$$

$$= \frac{2\hbar^2 A^2\Gamma\left(\frac{3}{2}\right)}{2A^{3/2}} = \frac{\hbar^2}{2}\sqrt{\pi A},$$

$$\langle V\rangle = \int_{-\infty}^{\infty} V(x)|\psi|^2\, dx = B\int_{-\infty}^{\infty} |x| e^{-Ax^2}\, dx = 2B\int_0^{\infty} xe^{-Ax^2}\, dx = \frac{2B\Gamma(2)}{2A} = \frac{B}{A}.$$

We combine these to find the energy as a function of *A*, namely

$$E(A) = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{1}{\langle\psi|\psi\rangle}\left(\frac{1}{2m}\langle P^2\rangle + \langle V\rangle\right) = \sqrt{\frac{A}{\pi}}\left(\frac{\hbar^2}{4m}\sqrt{\pi A} + \frac{B}{A}\right) = \frac{\hbar^2 A}{4m} + \frac{B}{\sqrt{\pi A}}.$$

We now need to minimize this with respect to *A*, so we have

$$0 = \frac{d}{dA}E(A) = \frac{\hbar^2}{4m} - \frac{B}{2\sqrt{\pi}A^{3/2}},$$

$$A = \left(\frac{2mB}{\sqrt{\pi}\hbar^2}\right)^{2/3}.$$

Substituting this back into the original formula, we have

$$E_{\min} = \frac{\hbar^2}{4m}\left(\frac{2mB}{\sqrt{\pi}\hbar^2}\right)^{2/3} + \frac{B}{\sqrt{\pi}}\left(\frac{\sqrt{\pi}\hbar^2}{2mB}\right)^{1/3} = \frac{\hbar^{2/3}B^{2/3}}{\pi^{1/3}m^{1/3}}\left(\frac{2^{2/3}}{4} + \frac{1}{2^{1/3}}\right) = \frac{3}{2}\left(\frac{\hbar^2 B^2}{2\pi m}\right)^{1/3}.$$

5. [25] A particle of mass *m* lies in the 2D infinite square square well with allowed region $0<x<a$ and $0<y<a$. In addition, there is a perturbation $W(x,y)=\gamma\delta\left(x-\tfrac{1}{4}a\right)\delta\left(y-\tfrac{1}{4}a\right)$.

(a)[3] What are the exact eigenstates and energies in the limit of no perturbation, $\gamma = 0$?

The exact eigenstates are products of the 1D case, and their energies are sums of the respective energies, so we have

$$\phi_{np}(x,y)=\frac{2}{a}\sin\left(\frac{\pi nx}{a}\right)\sin\left(\frac{\pi py}{a}\right),\quad \varepsilon_{np}=\frac{\pi^2\hbar^2}{2ma^2}\left(n^2+p^2\right).$$

(b) [7] Find the ground state energy to first order in γ.

The ground state energy is just

$$E_{11}=\varepsilon_{11}+\langle\phi_{11}|W|\phi_{11}\rangle=\frac{2\pi^2\hbar^2}{2ma^2}+\gamma\left(\frac{2}{a}\right)^2\int\sin^2\left(\frac{\pi x}{a}\right)\sin^2\left(\frac{\pi y}{a}\right)\delta\left(x-\frac{a}{4}\right)\delta\left(y-\frac{a}{4}\right)dx\,dy$$

$$=\frac{\pi^2\hbar^2}{ma^2}+\frac{4\gamma}{a^2}\sin^2\left(\frac{\pi}{4}\right)\sin^2\left(\frac{\pi}{4}\right)=\frac{\pi^2\hbar^2}{ma^2}+\frac{4\gamma}{a^2}\left(\frac{1}{\sqrt{2}}\right)^4=\frac{\pi^2\hbar^2}{ma^2}+\frac{\gamma}{a^2}.$$

(c) [15] For the first excited states, find the eigenstates to leading (zeroth) order and energies to first order.

The first excited states are $|\psi_{12}\rangle$ and $|\psi_{21}\rangle$, which are degenerate, and therefore we need to use degenerate perturbation theory and calculate what I call the $\tilde{W}$ matrix. Its components are

$$\langle\phi_{12}|W|\phi_{12}\rangle=\gamma\left(\frac{2}{a}\right)^2\int\sin^2\left(\frac{\pi x}{a}\right)\sin^2\left(\frac{2\pi y}{a}\right)\delta\left(x-\frac{a}{4}\right)\delta\left(y-\frac{a}{4}\right)dx\,dy$$

$$=\frac{4\gamma}{a^2}\sin^2\left(\frac{\pi}{4}\right)\sin^2\left(\frac{\pi}{2}\right)=\frac{4\gamma}{a^2}\left(\frac{1}{\sqrt{2}}\right)^2=\frac{2\gamma}{a^2},$$

$$\langle\phi_{12}|W|\phi_{21}\rangle=\gamma\left(\frac{2}{a}\right)^2\int\sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{2\pi x}{a}\right)\sin\left(\frac{2\pi y}{a}\right)\sin\left(\frac{\pi y}{a}\right)\delta\left(x-\frac{a}{4}\right)\delta\left(y-\frac{a}{4}\right)dx\,dy$$

$$=\frac{4\gamma}{a^2}\sin^2\left(\frac{\pi}{4}\right)\sin^2\left(\frac{\pi}{2}\right)=\frac{4\gamma}{a^2}\left(\frac{1}{\sqrt{2}}\right)^2=\frac{2\gamma}{a^2}=\langle\phi_{21}|W|\phi_{12}\rangle,$$

$$\langle\phi_{21}|W|\phi_{21}\rangle=\gamma\left(\frac{2}{a}\right)^2\int\sin^2\left(\frac{2\pi x}{a}\right)\sin^2\left(\frac{\pi y}{a}\right)\delta\left(x-\frac{a}{4}\right)\delta\left(y-\frac{a}{4}\right)dx\,dy$$

$$=\frac{4\gamma}{a^2}\sin^2\left(\frac{\pi}{2}\right)\sin^2\left(\frac{\pi}{4}\right)=\frac{4\gamma}{a^2}\left(\frac{1}{\sqrt{2}}\right)^2=\frac{2\gamma}{a^2}.$$

We therefore have

$$\tilde{W} = \frac{2\gamma}{a^2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}.$$

It is not hard to find the eigenvalues of the matrix without the factor out front using the characteristic equation:

$$0 = \det\begin{pmatrix} 1-\lambda & 1 \\ 1 & 1-\lambda \end{pmatrix} = (1-\lambda)^2 - 1 = -2\lambda + \lambda^2 = \lambda(\lambda - 2).$$

The full $\tilde{W}$ matrix then has eigenvalues of 0 and $4\gamma/a^2$. The corresponding states are pretty easily found; they are given below and have the corresponding energies:

$$E_1 = \frac{\pi^2\hbar^2}{2ma^2}\left(1^2+2^2\right) + \frac{4\gamma}{a^2} = \frac{5\pi^2\hbar^2}{2ma^2} + \frac{4\gamma}{a^2}, \quad |\psi_1\rangle = \frac{1}{\sqrt{2}}\left(|\phi_{12}\rangle + |\phi_{21}\rangle\right),$$
$$E_2 = \frac{\pi^2\hbar^2}{2ma^2}\left(1^2+2^2\right) + 0 = \frac{5\pi^2\hbar^2}{2ma^2}, \quad |\psi_2\rangle = \frac{1}{\sqrt{2}}\left(|\phi_{12}\rangle - |\phi_{21}\rangle\right).$$

6. **[15] Suppose we model a hydrogen atom as an electron orbiting a nucleus that produces a Coulomb potential given by $V(r) = -\frac{k_e e^2}{r}\left(1 - e^{-r/R}\right)$, where *R* is the nuclear size.**

   (a) **[4] If we compare this to the standard assumption that the nucleus has zero size, what is the perturbation *W* introduced by using a finite size?**

We normally assume a Hamiltonian for hydrogen of $H_0 = P^2/2m - k_e e^2/r$, but now we have $H = P^2/2m + V(r)$, so we must have $W = H - H_0 = V(r) + k_e e^2/r$, so we have

$$W = V(r) + \frac{k_e e^2}{r} = -\frac{k_e e^2}{r}\left(1 - e^{-r/R}\right) + \frac{k_e e^2}{r} = \frac{k_e e^2}{r}e^{-r/R}.$$

   (b) **[11] Assume the unperturbed wave function $\psi_{nlm}(\mathbf{r})$ is slowly varying over the nuclear scale. Estimate the energy shift ε' due to finite nuclear size in terms of $\psi_{nlm}(\mathbf{r})$. For which values of *n*, *l*, and *m* will the result be non-zero?**

To first order in the perturbation, the shift in energy is

$$\varepsilon'_{nlm} = \langle \psi_{nlm}|W|\psi_{nlm}\rangle = k_e e^2 \int \frac{1}{r}e^{-r/R}\left|\psi_{nlm}(\mathbf{r})\right|^2 d^3\mathbf{r}$$

Now, if *R* is much smaller than the atomic size, the wave function $\psi_{nlm}(\mathbf{r})$ will hardly vary over this volume, so we can treat it as constant. Taking it outside the integral, we have

$$\varepsilon'_{nlm} = k_e e^2\left|\psi_{nlm}(0)\right|^2 \int \frac{1}{r}e^{-r/R}d^3\mathbf{r} = k_e e^2\left|\psi_{nlm}(0)\right|^2 \int_0^\infty \frac{1}{r}e^{-r/R}r^2 dr \int d\Omega$$
$$= 4\pi k_e e^2\left|\psi_{nlm}(0)\right|^2 \int_0^\infty e^{-r/R} r\,dr = 4\pi k_e e^2\left|\psi_{nlm}(0)\right|^2 R^2\Gamma(2) = 4\pi k_e e^2 R^2\left|\psi_{nlm}(0)\right|^2.$$

The wave function vanishes at the origin except for when $l = 0$ (which implies that also $m = 0$). In this case, the angular wave function is just $1/\sqrt{4\pi}$, so we can write our answer in terms of just the radial wave function, so

$$\varepsilon'_{n00} = k_e e^2 R^2 R_{n0}^2(0).$$

Possibly Helpful Formulas:

Heisenberg Picture	**State Operators**	**1D Infinite Square Well**	**Spin Commutators**

Possibly Helpful Integrals: In the equations below A and B are positive.

$$\int_0^\infty x^n e^{-Ax} dx = \frac{\Gamma(n+1)}{A^{n+1}}, \quad \int_0^\infty x^n e^{-Ax^2} dx = \frac{\Gamma\left(\frac{n+1}{2}\right)}{2A^{\frac{n+1}{2}}}, \quad \Gamma(n) = (n-1)! \text{ if } n \text{ is an integer}, \quad \Gamma\left(\tfrac{1}{2}\right) = \sqrt{\pi}, \quad \Gamma\left(\tfrac{3}{2}\right) = \tfrac{1}{2}\sqrt{\pi}, \quad \Gamma\left(\tfrac{5}{2}\right) = \tfrac{3}{4}\sqrt{\pi},$$

$$\int \sqrt{A - B^2 x^2}\, dx = \frac{A}{2B} \sin^{-1}\left(\frac{Bx}{\sqrt{A}}\right) + \frac{x}{2}\sqrt{A - B^2 x^2}$$