Physics 742 – Graduate Quantum Mechanics 2

Solutions to First Exam, Spring 2024

Please note that some possibly helpful formulas are listed below or on the handout. The value of each question is listed in square brackets at the start of the problem or part.

1. [20] A spin-½ particle is in the spin state $|\psi_\phi\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ e^{i\phi}\end{pmatrix}$**, but the phase** ϕ **is randomly chosen in the range** $0<\phi<\pi$**. Note that the Pauli matrices** σ_i **are given in the equations.**

(a) [7] What is the state operator ρ**? Check that the trace has the correct value.**

If were in a definite state, we would have

$$\rho(\phi) = |\psi_\phi\rangle\langle\psi_\phi| = \frac{1}{2}\begin{pmatrix}1\\ e^{i\phi}\end{pmatrix}\begin{pmatrix}1 & e^{-i\phi}\end{pmatrix} = \frac{1}{2}\begin{pmatrix}1 & e^{-i\phi}\\ e^{i\phi} & 1\end{pmatrix}.$$

But because the angle is not known, we have to average over these angles, so we have

$$\rho = \frac{1}{\pi}\int_0^{\phi}\rho(\phi)\,d\phi = \frac{1}{2\pi}\int_0^{\pi}\begin{pmatrix}1 & e^{-i\phi}\\ e^{i\phi} & 1\end{pmatrix}d\phi = \frac{1}{2\pi}\begin{pmatrix}\phi & ie^{-i\phi}\\ -ie^{i\phi} & \phi\end{pmatrix}_0^{\pi} = \frac{1}{2\pi}\begin{pmatrix}\pi-0 & i\left(e^{-i\pi}-1\right)\\ -i\left(e^{i\pi}-1\right) & \pi-0\end{pmatrix}$$

$$= \frac{1}{2\pi}\begin{pmatrix}\pi & -2i\\ 2i & \pi\end{pmatrix}.$$

The trace is, of course, just one.

(b) [7] What would the expectation value of each of the three spin operators $S_i = \frac{1}{2}\hbar\sigma_i$ **?**

We use the general formulas, which is $\langle S_i\rangle = \mathrm{Tr}(\rho S_i) = \frac{1}{2}\hbar\,\mathrm{Tr}(\rho\sigma_i)$, which works out to

$$\langle S_x\rangle = \frac{\hbar}{2}\mathrm{Tr}(\rho\sigma_x) = \frac{\hbar}{2}\cdot\frac{1}{2\pi}\mathrm{Tr}\left(\begin{pmatrix}\pi & -2i\\ 2i & \pi\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\right) = \frac{\hbar}{4\pi}\mathrm{Tr}\begin{pmatrix}-2i & \pi\\ \pi & 2i\end{pmatrix} = 0,$$

$$\langle S_x\rangle = \frac{\hbar}{2}\mathrm{Tr}(\rho\sigma_x) = \frac{\hbar}{2}\cdot\frac{1}{2\pi}\mathrm{Tr}\left(\begin{pmatrix}\pi & -2i\\ 2i & \pi\end{pmatrix}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}\right) = \frac{\hbar}{4\pi}\mathrm{Tr}\begin{pmatrix}2 & -\pi i\\ \pi i & 2\end{pmatrix} = \frac{4\hbar}{4\pi} = \frac{\hbar}{\pi},$$

$$\langle S_z\rangle = \frac{\hbar}{2}\mathrm{Tr}(\rho\sigma_z) = \frac{\hbar}{2}\cdot\frac{1}{2\pi}\mathrm{Tr}\left(\begin{pmatrix}\pi & -2i\\ 2i & \pi\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\right) = \frac{\hbar}{4\pi}\mathrm{Tr}\begin{pmatrix}\pi & 2i\\ 2i & -\pi\end{pmatrix} = 0.$$

(c) [6] True or false: If the Hamiltonian is $H = \omega S_y$, the state operator is independent of time.

We use the formula given, namely

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

$$= \frac{\hbar\omega}{4\pi}\left\{\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}\begin{pmatrix}\pi & -2i\\ 2i & \pi\end{pmatrix} - \begin{pmatrix}\pi & -2i\\ 2i & \pi\end{pmatrix}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}\right\} = \frac{\hbar\omega}{4\pi}\left\{\begin{pmatrix}2 & -i\pi\\ i\pi & 2\end{pmatrix} - \begin{pmatrix}2 & -i\pi\\ i\pi & 2\end{pmatrix}\right\} = 0.$$

We see that the derivative vanishes, and hence it doesn't change.

2. [20] This problem should be worked entirely in terms of the Heisenberg formulation. A particle of mass *m* in one dimension has Hamiltonian $H = P^2/2m - FX$.

(a) [7] Find in this formalism equations for the time derivatives $\frac{d}{dt}X(t)$ and $\frac{d}{dt}P(t)$.

The equation for the time derivative is given so we have

$$\frac{d}{dt}X = \frac{i}{\hbar}[H,X] = \frac{i}{\hbar}\left[\frac{1}{2m}P^2 - FX, X\right] = \frac{i}{2m\hbar}\left[P^2, X\right] = \frac{i}{2m\hbar}\big(P[P,X] + [P,X]P\big)$$

$$= \frac{i(-i\hbar)}{2m\hbar}(P+P) = \frac{P}{m},$$

$$\frac{d}{dt}P = \frac{i}{\hbar}[H,P] = \frac{i}{\hbar}\left[\frac{1}{2m}P^2 - FX, P\right] = \frac{-iF}{\hbar}[X,P] = \frac{-iF}{\hbar}(i\hbar) = F.$$

(b) [6] Find $P(t)$ in terms of *P*(0) and *t*. Then find *X*(*t*) in terms of *X*(0), *P*(0) and *t*.

Since the derivative of P is a constant, its integral is a simple linear function, namely

$$P(t) = P(0) + Ft.$$

The constant of integration is chosen to be $P(0)$ so that it has the right value at $t = 0$. We now substitute this into the other equation to find

$$\frac{d}{dt}X = \frac{1}{m}P = \frac{P(0)}{m} + \frac{F}{m}t.$$

We simply integrate this to give

$$X(t) = X(0) + P(0)\frac{t}{m} + \frac{Ft^2}{2m}$$

(c) [7] Show that there is a lower limit on the uncertainties $\left[\Delta x(t)\right]\left[\Delta x(0)\right] \geq Ct$, and find *C*.

According to the generalized uncertainty principle,

$$\left[\Delta x(t)\right]\left[\Delta x(0)\right] \geq \frac{1}{2}\left|i\left\langle\left[X(t), X(0)\right]\right\rangle\right| = \frac{1}{2}\left|i\left\langle\left[X(0)+\frac{1}{m}P(0)t+\frac{F}{2m}t^2, X(0)\right]\right\rangle\right|$$

$$= \frac{1}{2m}\left|it\left\langle\left[P(0), X(0)\right]\right\rangle\right| = \frac{1}{2m}\left|it\left\langle -i\hbar\right\rangle\right| = \frac{\hbar|t|}{2m}.$$

Assuming *t* is positive, this is identical with the form requested.

3. [15] A particle of mass *m* in one dimension is in the potential $V(x) = \begin{cases} -\alpha x & x<0, \\ \beta x & x>0. \end{cases}$ Using the WKB method, estimate the energy of the *n*'th eigenstate.

We set the energy to *E*, and solve the equation $V(x) = E$ to find the two limits, which work out to

$$E = V(a) = -\alpha a, \quad a = -E/\alpha,$$
$$E = V(b) = \beta a, \quad b = E/\beta.$$

We then set up the WKB integral, and use the integral given in the table of integrals. We will have to split the integral into two regions. We have

$$\pi\hbar\left(n+\tfrac{1}{2}\right) = \int_a^b dx\sqrt{2m\left[E-V(x)\right]} = \int_{-E/\alpha}^0 dx\sqrt{2m(E+\alpha x)} + \int_0^{E/\beta} dx\sqrt{2m(E-\beta x)}$$

$$= \frac{\sqrt{2m}}{\alpha\frac{3}{2}}(E+\alpha x)^{3/2}\Big|_{-E/\alpha}^0 + \frac{\sqrt{2m}}{-\beta\frac{3}{2}}(E-\beta x)^{3/2}\Big|_0^{E/\beta} = \frac{2\sqrt{2m}}{3\alpha}\left(E^{3/2}-0\right) - \frac{2\sqrt{2m}}{3\beta}\left(0-E^{3/2}\right)$$

$$= \frac{2\sqrt{2m}}{3}E^{3/2}\left(\frac{1}{\alpha}+\frac{1}{\beta}\right).$$

We now solve this for *E* to yield

$$E^{3/2} = \frac{3\pi\hbar\left(n+\frac{1}{2}\right)}{2\sqrt{2m}\left(\alpha^{-1}+\beta^{-1}\right)},$$

$$E = \left[\frac{3\pi\hbar\left(n+\frac{1}{2}\right)}{2\sqrt{2m}\left(\alpha^{-1}+\beta^{-1}\right)}\right]^{2/3}.$$

4. [15] A particle of mass *m* lies in the potential $V(x) = B|x|^3$. Estimate the energy of the ground state energy by the variational method using the trial wave function $\psi(x) = e^{-\alpha x^2/2}$.

We need to calculate three quantities: the expectation of the momentum squared, the potential, and the normalization of the wave function. Everything is even, so we can integrate only for $x > 0$ and double the results. We have

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

$$\langle\psi|P^2|\psi\rangle = \|P|\psi\rangle\|^2 = \int_{-\infty}^{\infty} \left|-i\hbar\frac{d}{dx}\psi(x)\right|^2 dx = 2\hbar^2\int_0^\infty \left[\frac{d}{dx}e^{-\alpha x^2/2}\right]^2 dx = 2\hbar^2\int_0^\infty \left(-\alpha x e^{-\alpha x^2/2}\right)^2 dx$$

$$= 2\hbar^2\alpha^2\int_0^\infty x^2 e^{-Ax^2} dx = \frac{2\hbar^2\alpha^2\Gamma\left(\frac{3}{2}\right)}{2\alpha^{3/2}} = \hbar^2\sqrt{a}\,\tfrac{1}{2}\sqrt{\pi} = \tfrac{1}{2}\hbar^2\sqrt{\pi a},$$

$$\langle\psi|V(x)|\psi\rangle = \int_{-\infty}^{\infty} |\psi(x)|^2 dx = 2B\int_0^\infty x^3\left(e^{-\alpha x^2/2}\right)^2 dx = 2B\int_0^\infty x^3 e^{-\alpha x^2} dx = \frac{2B\Gamma(2)}{2\alpha^2} = \frac{B}{\alpha^2}.$$

We now put this into the energy formula which gives us

$$E(A) = \frac{1}{\langle\psi|\psi\rangle}\left(\frac{1}{2m}\langle P^2\rangle + \langle V\rangle\right) = \sqrt{\frac{\alpha}{\pi}}\left(\frac{\hbar^2\sqrt{\pi\alpha}}{4m} + \frac{B}{\alpha^2}\right) = \frac{\hbar^2\alpha}{4m} + \frac{B}{\sqrt{\pi}\alpha^{3/2}}.$$

We now need to minimize this, which we set to zero, and we find

$$0 = \frac{d}{d\alpha}E(\alpha) = \frac{\hbar^2}{4m} - \frac{3B}{2\sqrt{\pi}\alpha^{5/2}},$$

$$2\sqrt{\pi}\hbar^2\alpha^{5/2} = 12mB,$$

$$\alpha^{5/2} = \frac{6mB}{\hbar^2\sqrt{\pi}},$$

$$\alpha = \left(\frac{6mB}{\hbar^2\sqrt{\pi}}\right)^{2/5}.$$

Substituting this value of *A* back into the formula, we have

$$E(A) = \frac{\hbar^2}{4m}\left(\frac{6mB}{\hbar^2\sqrt{\pi}}\right)^{2/5} + \frac{B}{\sqrt{\pi}}\left(\frac{\hbar^2\sqrt{\pi}}{6mB}\right)^{3/5} = \left(\frac{6B\hbar^3}{m\sqrt{\pi m}}\right)^{2/5}\left(\frac{1}{4} + \frac{1}{6}\right) = \frac{5}{12}\left(\frac{6B\hbar^3}{m\sqrt{\pi m}}\right)^{2/5}.$$

5. **[15] 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 small perturbation of the form $W(x,y) = \lambda\cos(\pi x/a)\cos(\pi y/a)$, where λ is small.**

   (a)[2] What are the exact eigenstates and energies in the limit of no perturbation, λ = 0?

The eigenstates are products of eigenstates in each of the two dimensions, so we have

$$\phi_{nm}(x,y) = \frac{2}{a}\sin\left(\frac{\pi nx}{a}\right)\sin\left(\frac{\pi my}{a}\right),$$
$$\varepsilon_{nm} = \frac{\pi^2\hbar^2 n^2}{2ma^2} + \frac{\pi^2\hbar^2 m^2}{2ma^2} = \frac{\pi^2\hbar^2\left(n^2+m^2\right)}{2ma^2}.$$

   (b) [13] Find the ground state wave function to first order and the energy to second order in λ.

The eigenstates to first order and energies to second order will be

$$|\psi_{11}\rangle = |\phi_{11}\rangle + \sum_{nm\neq 11} |\phi_{nm}\rangle \frac{\langle\phi_{nm}|W|\phi_{11}\rangle}{\varepsilon_{11}-\varepsilon_{nm}}, \quad E_{11} = \varepsilon_{11} + \langle\phi_{11}|W|\phi_{11}\rangle + \sum_{nm\neq 11}\frac{\left|\langle\phi_{nm}|W|\phi_{11}\rangle\right|^2}{\varepsilon_{11}-\varepsilon_{nm}}.$$

We therefore need the matrix elements

$$\langle\phi_{nm}|W|\phi_{11}\rangle = \int_0^a dx\int_0^a dy\,\frac{2}{a}\sin\left(\frac{\pi nx}{a}\right)\sin\left(\frac{\pi my}{a}\right)\lambda\cos\left(\frac{\pi x}{a}\right)\cos\left(\frac{\pi y}{a}\right)\frac{2}{a}\sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{\pi y}{a}\right)$$
$$= \frac{4\lambda}{a^2}\cdot\frac{a}{4}\left(\delta_{1+1,n}+\delta_{n+1,1}-\delta_{n+1,1}\right)\cdot\frac{a}{4}\left(\delta_{1+1,m}+\delta_{m+1,1}-\delta_{m+1,1}\right) = \frac{\lambda}{4}\delta_{2,n}\delta_{2,m}.$$

The delta functions then assure that there will only be one term in the sums. For the state, we have

$$|\psi_{11}\rangle = |\phi_{11}\rangle + |\phi_{22}\rangle\frac{\langle\phi_{22}|W|\phi_{11}\rangle}{\varepsilon_{11}-\varepsilon_{22}} = |\phi_{11}\rangle + |\phi_{22}\rangle\frac{\lambda/4}{\left(\pi^2\hbar^2/2ma^2\right)(1+1-4-4)} = |\phi_{11}\rangle - \frac{\lambda ma^2}{12\pi^2\hbar^2}|\phi_{22}\rangle.$$

Since the problem asks for the wave functions, we simply substitute them in to get

$$\psi_{11}(x,y) = \frac{2}{a}\sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{\pi y}{a}\right) - \frac{\lambda ma}{6\pi^2\hbar^2}\sin\left(\frac{2\pi x}{a}\right)\sin\left(\frac{2\pi y}{a}\right).$$

For the energy, we have

$$E_{11} = \varepsilon_{11} + \langle\phi_{11}|W|\phi_{11}\rangle + \frac{\left|\langle\phi_{22}|W|\phi_{11}\rangle\right|^2}{\varepsilon_{11}-\varepsilon_{22}} = \frac{\pi^2\hbar^2 2}{2ma^2} + 0 + \frac{(\lambda/4)^2}{\left(\pi^2\hbar^2/2ma^2\right)(1+1-4-4)}$$
$$= \frac{\pi^2\hbar^2}{ma^2} + \frac{\lambda^2 2ma^2}{16\pi^2\hbar^2(-6)} = \frac{\pi^2\hbar^2}{ma^2} - \frac{\lambda^2 ma^2}{48\pi^2\hbar^2}.$$

6. **[15] An electron is trapped in a Coulomb potential of the form $V_C(\mathbf{r}) = Ar$. It is in one of the *l* = 1 states, so its space wave function looks like $\psi(\mathbf{r}) = R(r)Y_1^m(\theta,\phi)$ where $Y_1^m(\theta,\phi)$ is a spherical harmonic and $R(r)$ is a radial wave function.**

   (a) [8] Given that *l* = 1, what are the possible values of *j*, the total angular momentum quantum number? For each of these values of *j*, work out the corresponding eigenvalue of $\mathbf{L}\cdot\mathbf{S}$.

The values of *j* go from $j = |l-s|$ to $j = l+s$ in steps of size 1. Since $l = 1$ and $s = \frac{1}{2}$, the only possible values of *j* are $j = \frac{1}{2}$ and $j = \frac{3}{2}$.

To find the corresponding eigenvalue of $\mathbf{L}\cdot\mathbf{S}$, we use the trick

$$\mathbf{L}\cdot\mathbf{S} = \tfrac{1}{2}(\mathbf{L}+\mathbf{S})^2 - \tfrac{1}{2}\mathbf{L}^2 - \tfrac{1}{2}\mathbf{S}^2 = \tfrac{1}{2}\mathbf{J}^2 - \tfrac{1}{2}\mathbf{L}^2 - \tfrac{1}{2}\mathbf{S}^2 = \tfrac{1}{2}\hbar^2\left(j^2 + j - 1 - 1 - \tfrac{1}{4} - \tfrac{1}{2}\right) = \tfrac{1}{2}\hbar^2\left(j^2 + j - \tfrac{11}{4}\right)$$

This works out to:

$$j = \tfrac{1}{2}: \quad \mathbf{L}\cdot\mathbf{S} = \tfrac{1}{2}\hbar^2\left(\tfrac{1}{4} + \tfrac{1}{2} - \tfrac{11}{4}\right) = -\hbar^2 ,$$
$$j = \tfrac{3}{2}: \quad \mathbf{L}\cdot\mathbf{S} = \tfrac{1}{2}\hbar^2\left(\tfrac{9}{4} + \tfrac{3}{2} - \tfrac{11}{4}\right) = \tfrac{1}{2}\hbar^2 .$$

   (b) [7] Find the energy splitting $\Delta\varepsilon'$ between the different states you found in part (a) due to spin-orbit coupling. Since you don't know the radial wave function, you will have to leave one integral undone.

If we label our states as $|n,l,j,m_j\rangle$, then the splitting will be

$$\begin{aligned}
\Delta E = \varepsilon'_{3/2} - \varepsilon'_{1/2} &= \left\langle n,1,\tfrac{3}{2},m_j \middle| W_{SO} \middle| n,1,\tfrac{3}{2},m_j \right\rangle - \left\langle n,1,\tfrac{1}{2},m_j \middle| W_{SO} \middle| n,1,\tfrac{1}{2},m_j \right\rangle \\
&= \hbar^2\left(\tfrac{1}{2} - (-1)\right)\left\langle \psi \middle| \frac{g}{4m^2c^2}\frac{1}{r}\frac{dV_c(r)}{dr} \middle| \psi \right\rangle = \frac{3\hbar^2}{2}\frac{gA}{4m^2c^2}\left\langle \psi \middle| \frac{1}{r} \middle| \psi \right\rangle \\
&= \frac{3\hbar^2 gA}{8m^2c^2}\int Y_1^{m*}(\theta,\phi)Y_1^m(\theta,\phi)\,d\Omega\int_0^\infty \frac{1}{r}r^2R^2(r)\,dr = \frac{3\hbar^2 gA}{8m^2c^2}\int_0^\infty rR^2(r)\,dr
\end{aligned}$$

As it says in the problem, we can't do the final integral.

Possibly Helpful Formulas:

Pauli Matrices	Heisenberg Picture	1D Infinite Square Well
$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$\frac{d}{dt}A(t) = \frac{i}{\hbar}\left[H(t), A(t)\right]$	$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{\pi n x}{a}\right)$
$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$	**Spin-Orbit Coupling**	$E_n = \frac{\pi^2\hbar^2 n^2}{2ma^2}$
$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$W_{\mathrm{SO}} = \frac{g}{4m^2c^2}\frac{1}{r}\frac{dV_c(r)}{dr}\mathbf{L}\cdot\mathbf{S}$	**Generalized Uncertainty**
		$(\Delta a)(\Delta b) \ge \frac{1}{2}\left|\left\langle i[A,B]\right\rangle\right|$

State Operators

$$i\hbar\frac{d}{dt}\rho = [H,\rho]$$

Possibly Helpful Integrals:

In the equations below A is positive, and in the last equation n, m and p are positive integers.

$$\int (ax+b)^n\,dx = \frac{1}{a(n+1)}(ax+b)^{n+1}$$

$$\int_0^\infty x^n e^{-Ax^2}\,dx = \frac{1}{2A^{(n+1)/2}}\Gamma\left(\frac{n+1}{2}\right), \quad \Gamma(1) = \Gamma(2) = 1, \quad \Gamma\left(\tfrac{1}{2}\right) = \sqrt{\pi}, \quad \Gamma\left(\tfrac{3}{2}\right) = \tfrac{1}{2}\sqrt{\pi}.$$

$$\int_0^a \sin\left(\frac{\pi n x}{a}\right)\sin\left(\frac{\pi m x}{a}\right)\cos\left(\frac{\pi p x}{a}\right)dx = \frac{a}{4}\left(\delta_{n,m+p} + \delta_{m,n+p} - \delta_{p,n+m}\right).$$