Physics 742 – Graduate Quantum Mechanics 2

Solutions to Midterm Exam, Spring 2021

Please note that some possibly helpful formulas are listed on the next page. Each question is worth twenty points. The points for individual parts are marked in []'s.

1. A spin ½ particle has state operator given by $\rho = N\begin{pmatrix} 2 & 1+i \\ c & 2 \end{pmatrix}$**, where** N **and** c **are constants.**

(a) [5] What is the normalization constant N**? What is the complex number** c**?**

The state operator must be Hermitian and have trace 1. The trace is $\mathrm{Tr}(\rho) = 4N = 1$, so $N = \frac{1}{4}$. To be Hermitian, we must have $c = 1-i$. We note that the resulting state operator is

$$\rho = \frac{1}{4}\begin{pmatrix} 2 & 1+i \\ 1-i & 2 \end{pmatrix} = \tfrac{1}{2}\mathbf{1} + \tfrac{1}{4}\sigma_x - \tfrac{1}{4}\sigma_y .$$

The Pauli matrices σ_i are the spin matrices listed below with the factor of $\frac{1}{2}\hbar$ removed, and $\mathbf{1}$ is the identity matrix.

(b) [15] What are the expectation values of each of the three spin operators S (given below)?

$$S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad S_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The expectation value of any operator A is given by $\mathrm{Tr}(\rho A)$. We now take advantage of the fact that $\mathrm{Tr}(\sigma_i) = 0$ and $\mathrm{Tr}(\sigma_i \sigma_j) = 2\delta_{ij}$, so that we have

$$\langle S_x \rangle = \tfrac{1}{2}\hbar \mathrm{Tr}\left[\sigma_x\left(\tfrac{1}{2}\mathbf{1} + \tfrac{1}{4}\sigma_x - \tfrac{1}{4}\sigma_y\right)\right] = \tfrac{1}{8}\hbar \mathrm{Tr}\left(2\sigma_x + \sigma_x\sigma_x - \sigma_x\sigma_y\right) = \tfrac{1}{4}\hbar,$$
$$\langle S_y \rangle = \tfrac{1}{2}\hbar \mathrm{Tr}\left[\sigma_y\left(\tfrac{1}{2}\mathbf{1} + \tfrac{1}{4}\sigma_x - \tfrac{1}{4}\sigma_y\right)\right] = \tfrac{1}{8}\hbar \mathrm{Tr}\left(2\sigma_y + \sigma_y\sigma_x - \sigma_y\sigma_y\right) = -\tfrac{1}{4}\hbar,$$
$$\langle S_z \rangle = \tfrac{1}{2}\hbar \mathrm{Tr}\left[\sigma_z\left(\tfrac{1}{2}\mathbf{1} + \tfrac{1}{4}\sigma_x - \tfrac{1}{4}\sigma_y\right)\right] = \tfrac{1}{8}\hbar \mathrm{Tr}\left(2\sigma_z + \sigma_z\sigma_x - \sigma_z\sigma_y\right) = 0.$$

2. A particle of mass *m* in <u>two</u> dimensions lies in a potential $V = -V_0 e^{-\beta\rho^2}$. Estimate the energy of the ground state using the trial wave function $\psi = e^{-\alpha\rho^2/2}$.

We need to compute the following three quantities:

$$\langle\psi|\psi\rangle = \int d^2\mathbf{r}\left|\psi(\mathbf{r})\right|^2 = \int_0^{2\pi} d\phi\int_0^\infty e^{-\alpha\rho^2}\rho\,d\rho = 2\pi\cdot\tfrac{1}{2}\alpha^{-1}\Gamma(1) = \frac{\pi}{\alpha},$$

$$\langle V\rangle = \int d^2\mathbf{r}\,V(\mathbf{r})\left|\psi(\mathbf{r})\right|^2 = -V_0\int_0^{2\pi} d\phi\int_0^\infty e^{-\alpha\rho^2}e^{-\beta\rho^2}\rho\,d\rho = -2\pi V_0\cdot\tfrac{1}{2}(\alpha+\beta)^{-1}\Gamma(1) = -\frac{\pi V_0}{\alpha+\beta},$$

$$\langle\mathbf{P}^2\rangle = \left|\mathbf{P}|\psi\rangle\right|^2 = \int d^2\mathbf{r}\left|-i\hbar\nabla\psi(\mathbf{r})\right|^2 = \hbar^2\int_0^{2\pi} d\phi\int_0^\infty \left|\nabla e^{-\alpha\rho^2/2}\right|^2\rho\,d\rho$$

$$= 2\pi\hbar^2\int_0^\infty\left|-\alpha\rho\hat{\boldsymbol{\rho}}e^{-\alpha\rho^2/2}\right|^2\rho\,d\rho = 2\pi\hbar^2\alpha^2\int_0^\infty e^{-\alpha\rho^2}\rho^3\,d\rho = 2\pi\hbar^2\alpha^2\,\tfrac{1}{2}\alpha^{-2}\Gamma(2) = \pi\hbar^2.$$

We now put this together to get the energy expectation value as a function of the parameter α:

$$E(\alpha) = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{1}{\langle\psi|\psi\rangle}\left(\frac{1}{2m}\langle\mathbf{P}^2\rangle + \langle V\rangle\right) = \frac{\alpha}{\pi}\left(\frac{\pi\hbar^2}{2m} - \frac{\pi V_0}{\alpha+\beta}\right) = \frac{\hbar^2\alpha}{2m} - \frac{\alpha V_0}{\alpha+\beta}.$$

We want to minimize this quantity, so we take the derivative and set it equal to zero, which yields

$$0 = \frac{d}{d\alpha}E(\alpha) = \frac{\hbar^2}{2m} - \frac{V_0(\alpha+\beta-\alpha)}{(\alpha+\beta)^2} = \frac{\hbar^2}{2m} - \frac{V_0\beta}{(\alpha+\beta)^2},$$

$$\hbar^2(\alpha+\beta)^2 = 2mV_0\beta,$$

$$\alpha_{\min} = \frac{\sqrt{2mV_0\beta}}{\hbar} - \beta.$$

Substituting this into the expression for the energy, we have

$$E(\alpha_{\min}) = \frac{\hbar^2}{2m}\left(\frac{\sqrt{2mV_0\beta}}{\hbar} - \beta\right) - \frac{V_0\left(\hbar^{-1}\sqrt{2mV_0\beta} - \beta\right)}{\hbar^{-1}\sqrt{2mV_0\beta}} = \hbar\sqrt{\frac{V_0\beta}{2m}} - \frac{\beta\hbar^2}{2m} - V_0 + \hbar\sqrt{\frac{V_0\beta}{2m}}$$

$$E_g \approx 2\hbar\sqrt{\frac{V_0\beta}{2m}} - \frac{\beta\hbar^2}{2m} - V_0.$$

There is a technicality; namely, that our integrals assumed that $\alpha > 0$, which occurs only if $\sqrt{2mV_0/\beta} > \hbar$. If this isn't true, in fact this method fails to find *any* bound state.

3. In the basis $\{|\phi_1\rangle, |\phi_2\rangle, |\phi_3\rangle\}$, the Hamiltonian is given by $H = \begin{pmatrix} A & i\delta & 0 \\ -i\delta & 2A & \delta \\ 0 & \delta & 2A \end{pmatrix}$, with δ small.

(a) [2] What are the eigenstates and eigenenergies in the limit $\delta = 0$?

In this limit, the matrix is diagonal, so the states are $\{|\phi_1\rangle, |\phi_2\rangle, |\phi_3\rangle\}$ and the energies are $\varepsilon_1 = A$ and $\varepsilon_2 = \varepsilon_3 = 2A$. The perturbation is all the matrix with all the δ's.

(b) [8] For the ground state, what is the eigenstate to first order in δ and the energy to second order in δ?

The ground state is $|\phi_1\rangle$, which after including the perturbation would become

$$|\psi_1\rangle = |\phi_1\rangle + \sum_{m\neq 1} |\phi_m\rangle \frac{\langle \phi_m | W | \phi_1 \rangle}{\varepsilon_1 - \varepsilon_m} = |\phi_1\rangle + |\phi_2\rangle \frac{\langle \phi_2 | W | \phi_1 \rangle}{\varepsilon_1 - \varepsilon_2} = |\phi_1\rangle + \frac{-i\delta}{A - 2A} |\phi_2\rangle = |\phi_1\rangle + \frac{i\delta}{A} |\phi_2\rangle.$$

The energy is given by

$$E_1 = \varepsilon_1 + \langle \psi_1 | W | \psi_1 \rangle + \sum_{m\neq 1} \frac{\left|\langle \phi_m | W | \phi_1 \rangle\right|^2}{\varepsilon_1 - \varepsilon_m} = A + 0 + \frac{\left|\langle \phi_2 | W | \phi_1 \rangle\right|^2}{\varepsilon_1 - \varepsilon_2} = A + \frac{\left|-i\varepsilon\right|^2}{A - 2A} = A - \frac{\varepsilon^2}{A}.$$

(c) [10] For the first excited states, what are the eigenstates to leading order in δ and the energy to first order in δ?

For the first excited states, the states are degenerate, so we must use degenerate perturbation theory. The first step is to write the $\tilde{W}$ matrix, which is just the W matrix restricted to the two states $\{|\phi_2\rangle, |\phi_3\rangle\}$, which trivially is

$$\tilde{W} = \begin{pmatrix} 0 & \delta \\ \delta & 0 \end{pmatrix}.$$

This matrix comes up so often we should probably simply memorize the (normalized) eigenvectors, which will have eigenvectors and eigenvalues

$$|\psi_\pm\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix}, \quad \varepsilon' = \pm\delta.$$

Writing this in the given basis, and including the unperturbed energy, our states and energies are

$$|\psi_\pm\rangle = \tfrac{1}{\sqrt{2}}\left(|\phi_2\rangle \pm |\phi_2\rangle\right), \quad E'_\pm = 2A \pm \delta.$$

4. A particle of mass *m* lies in the 1D potential $V(x)=\begin{cases}\frac{1}{2}m\omega^2x^2-A & x>0,\\ \frac{1}{2}m\omega^2x^2 & x<0.\end{cases}$

Use the WKB approximation to estimate the energy of the *n*'th state (assume $E_n > 0$).

We need to first find the turning points, the two points where $V(x)=E$. We must solve it separately for $x>0$ and $x<0$. We have:

$$x<0:\quad E=\tfrac{1}{2}m\omega^2x^2,\quad x=-\sqrt{\frac{2E}{m\omega^2}},$$

$$x>0:\quad E=\tfrac{1}{2}m\omega^2x^2-A,\quad x=+\sqrt{\frac{2(E+A)}{m\omega^2}}.$$

We now substitute these two limits into our WKB integral. We must, of course, split the integral into two pieces, because the potential changes abruptly. We therefore have

$$\begin{aligned}\pi\hbar\left(n+\tfrac{1}{2}\right)&=\int_{-\sqrt{2E/m\omega^2}}^{\sqrt{2(E+A)/m\omega^2}}\sqrt{2m\left[E-V(x)\right]}\,dx\\ &=\int_{-\sqrt{2E/m\omega^2}}^{0}\sqrt{2m\left[E-\tfrac{1}{2}m\omega^2x^2\right]}\,dx+\int_0^{\sqrt{2(E+A)/m\omega^2}}\sqrt{2m\left[E-\tfrac{1}{2}m\omega^2x^2+A\right]}\,dx\\ &=\int_0^{\sqrt{2E/m\omega^2}}\sqrt{2mE-m^2\omega^2x^2}\,dx+\int_0^{\sqrt{2(E+A)/m\omega^2}}\sqrt{2m(E+A)-m^2\omega^2x^2}\,dx.\end{aligned}$$

We changed variables $x\to -x$ for the first term. Fortunately, this integral is given in the table, though it's a bit of a mess. We have

$$\begin{aligned}\pi\hbar\left(n+\tfrac{1}{2}\right)&=\int_0^{\sqrt{2E/m\omega^2}}\sqrt{2mE-m^2\omega^2x^2}\,dx+\int_0^{\sqrt{2(E+A)/m\omega^2}}\sqrt{2mE+2mA-m^2\omega^2x^2}\,dx\\ &=\left[\frac{2mE}{2\sqrt{m^2\omega^2}}\sin^{-1}\left(\sqrt{\frac{2E}{m\omega^2}}\sqrt{\frac{m^2\omega^2}{2mE}}\right)+\frac{1}{2}\sqrt{\frac{2E}{m\omega^2}}\sqrt{2mE-m^2\omega^2\frac{2E}{m\omega^2}}\right]\\ &\quad+\left[\frac{2m(E+A)}{2\sqrt{m^2\omega^2}}\sin^{-1}\left(\sqrt{\frac{2(E+A)}{m\omega^2}}\sqrt{\frac{m^2\omega^2}{2m(E+A)}}\right)+\frac{x}{2}\sqrt{2m(E+A)-m^2\omega^2\frac{2(E+A)}{m\omega^2}}\right]\\ &=\frac{E}{\omega}\sin^{-1}(1)+0+\frac{E+A}{\omega}\sin^{-1}(1)+0=\frac{\pi}{2}\cdot\frac{2E+A}{\omega}=\frac{\pi}{\omega}\left(E+\tfrac{1}{2}A\right),\end{aligned}$$

$$\pi\hbar\omega\left(n+\tfrac{1}{2}\right)=\pi\left(E+\tfrac{1}{2}A\right),$$

$$E_n=\hbar\omega\left(n+\tfrac{1}{2}\right)-\tfrac{1}{2}A.$$

We note that this works perfectly if $A = 0$, for which we have the harmonic oscillator.

5. **Imagine that a proton in a hydrogen atom consists of a point charge at the origin of magnitude $\frac{1}{2}e$ and a spherical shell of magnitude $\frac{1}{2}e$ at radius *R*.**

(a) **[12] Find the electric field for $r < R$ (the electric field from a point charge *q* is $E = k_e q r^{-2}$). Integrate it to find the electric potential $U(r) = -\int E\,dr$ in the interior region. Choose the constant of integration so $U(R) = k_e e R^{-1}$, as it must.**

The electric field from a spherically symmetric charge distribution always looks like a point charge whose magnitude includes *only* the charge that is closer than the point from which you are looking. For $r < R$, this will be $\frac{1}{2}e$, so the electric field will be $E = \frac{1}{2}k_e e r^{-2}$ For $r > R$, it is the whole charge, so $E = k_e e r^{-2}$. Integrating, we get the potential in each region:

$$U_>(r) = -\int E_>\,dr = -\int k_e e \frac{dr}{r^2} = \frac{k_e e}{r} + C_>, \quad r > R,$$
$$U_<(r) = -\int E_<\,dr = -\int \frac{k_e e}{2}\frac{dr}{r^2} = \frac{k_e e}{2r} + C_<, \quad r < R.$$

Because the potential at infinity must vanish, we see that $C_> = 0$, and therefore $U_>(R) = k_e e/R$. This must match the potential inside, which is $U_<(R) = k_e e/2R + C_<$. Equating these, we have $k_e e/2R + C_< = k_e e/R$, so that $C_< = k_e e/2R$. We therefore have, for the interior region,

$$U_<(r) = \frac{k_e e}{2r} + \frac{k_e e}{2R}, \quad r < R.$$

(b) **[3] Find the perturbation due to finite size, $W(r) = -eU(r) - \left(-k_e e^2 r^{-1}\right)$.**

This is trivial, since we are given the formula

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

Of course, this is only in the region $r < R$; for $r > R$, the potential vanishes.

(c) **[5] Find the shift in energy due to the finite proton size, assuming that in the nuclear region $\psi(\mathbf{r}) \approx \psi(0)$. You may leave your answers in terms of $\psi(0)$.**

We calculate the shift in energy using first-order perturbation theory:

$$\varepsilon' = \langle\psi|W(r)|\psi\rangle = \int|\psi(\mathbf{r})|^2 W(r)\,d^3\mathbf{r} \approx |\psi(0)|^2\int W(r)\,d^3\mathbf{r} = |\psi(0)|^2\int d\Omega\int_0^R r^2 W(r)\,dr$$
$$= 4\pi|\psi(0)|^2\frac{1}{2}k_e e^2\int_0^R r^2\left(\frac{1}{r} - \frac{1}{R}\right)dr = 2\pi k_e e^2|\psi(0)|^2\left(\frac{1}{2}R^2 - \frac{1}{3}R^2\right) = \frac{\pi}{3}k_e e^2 R^2|\psi(0)|^2.$$

Calculus in 2D:

$$\nabla\psi = \frac{\partial\psi}{\partial\rho}\hat{\boldsymbol{\rho}} + \frac{1}{\rho}\frac{\partial\psi}{\partial\phi}\hat{\boldsymbol{\varphi}}, \quad \nabla^2\psi = \frac{\partial^2\psi}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial\psi}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2\psi}{\partial\phi^2}, \quad \int f(\rho,\phi)\,d^2\mathbf{r} = \int_0^{2\pi} d\phi \int_0^\infty f(\rho,\phi)\,\rho\,d\rho$$

Possibly Helpful Integrals:

$$\int_0^\infty \rho^n e^{-A\rho^2}\,dx = \tfrac{1}{2}A^{-(n+1)/2}\Gamma\left(\tfrac{n+1}{2}\right), \quad \Gamma(1) = \Gamma(2) = 1, \quad \Gamma\left(\tfrac{1}{2}\right) = \sqrt{\pi}, \quad \Gamma\left(\tfrac{3}{2}\right) = \tfrac{1}{2}\sqrt{\pi}, \quad \Gamma\left(\tfrac{5}{2}\right) = \tfrac{3}{4}\sqrt{\pi}.$$

$$\int_0^y \sqrt{a-bx}\,dx = \frac{2}{3b}\left[a^{3/2} - (a-by)^{3/2}\right], \quad \int_0^y \sqrt{a-bx^2}\,dx = \frac{a}{2\sqrt{b}}\sin^{-1}\left(y\sqrt{b/a}\right) + \frac{y}{2}\sqrt{a-by^2}.$$