Physics 742 – Graduate Quantum Mechanics 2

Solutions to First Exam, Spring 2023

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. [10] A particle of mass *m* in one dimension is in the potential $V(x) = -\beta|x|^{-2/3}$. Using the WKB method, estimate the energy of the *n*'th eigenstate (the energies will be negative). I recommend making the substitution $x = y^{3/2}$ and then $z = \beta + Ey$.

The first step to using the WKB method is to find the turning points, the places where $V(x) = E$. Rearranging slightly, we see that $-E/\beta = |x|^{-2/3}$, so $|x| = (-\beta/E)^{3/2}$ with solution $x = \pm(-\beta/E)^{3/2}$. We use this as our limits of integration in the WKB formula, which yields

$$\pi\hbar\left(n+\tfrac{1}{2}\right) = \int_{-(-\beta/E)^{3/2}}^{(-\beta/E)^{3/2}} \sqrt{2m\left[E - V(x)\right]}dx = 2\int_0^{(-\beta/E)^{3/2}} \sqrt{2m\left(E + \beta x^{-2/3}\right)}dx,$$

where we have used the symmetric nature of the integral to switch it to just positive *x* and then get rid of the absolute values. We now use the two suggested substitutions to have

$$\pi\hbar\left(n+\tfrac{1}{2}\right) = 2\int_0^{-\beta/E} \sqrt{2m\left(E + \beta y^{-1}\right)}d\left(y^{3/2}\right) = 3\int_0^{-\beta/E} \sqrt{2m\left(E + \beta y^{-1}\right)}y^{1/2}dy$$

$$= 3\int_0^{-\beta/E} \sqrt{2m\left(Ey + \beta\right)}dy = \frac{3}{E}\int_\beta^0 \sqrt{2mz}dz = \frac{3\sqrt{2m}}{E}\frac{2}{3}z^{3/2}\Big|_\beta^0 = -\frac{2\sqrt{2m}}{E}\beta^{3/2}.$$

Solving for *E*, we have $E = -\dfrac{2\sqrt{2m\beta^3}}{\pi\hbar\left(n+\frac{1}{2}\right)}$.

2. [30] A particle of mass *m* in 3D is in the potential $V(x,y,z) = \frac{1}{2}m\omega^2\left(x^2+y^2+z^2\right) + \lambda xy$, where λ is small.

(a) [4] Name and give the energies of the eigenstates of the unperturbed Hamiltonian in the limit $\lambda = 0$.

(b) [13] For the ground state, find the state to first order in λ and the energy to second order in λ.

(c) [13] For the first excited states, find the states to leading order and energies to first order in λ.

This is just a 3D harmonic oscillator, with states

$$|mnp\rangle, \quad \text{with} \quad \varepsilon_{mnp} = \hbar\omega\left(n+m+p+\tfrac{3}{2}\right).$$

To find the state and energy to first order for the ground state, we introduce the perturbation $W = \lambda XY$. Letting this act on the ground state yields

$$W\left|000\right\rangle = \lambda XY\left|000\right\rangle = \lambda\left[\sqrt{\frac{\hbar}{2m\omega}}\left(a_x + a_x^\dagger\right)\right]\left[\sqrt{\frac{\hbar}{2m\omega}}\left(a_y + a_y^\dagger\right)\right]\left|000\right\rangle$$

$$= \frac{\lambda\hbar}{2m\omega}\left(a_x + a_x^\dagger\right)\left(a_y + a_y^\dagger\right)\left|000\right\rangle = \frac{\lambda\hbar}{2m\omega}\left(a_x + a_x^\dagger\right)\left|010\right\rangle = \frac{\lambda\hbar}{2m\omega}\left|110\right\rangle.$$

The energy of the ground state will therefore be to second order

$$E_{000} = \varepsilon_{000} + \left\langle 000\right|W\left|000\right\rangle + \sum_{mnp\neq 000}\frac{\left|\left\langle mnp\right|W\left|000\right\rangle\right|^2}{\varepsilon_{000} - \varepsilon_{mnp}} = \frac{3}{2}\hbar\omega + 0 + \left(\frac{\lambda\hbar}{2m\omega}\right)^2\frac{1}{-2\hbar\omega}$$

$$= \frac{3}{2}\hbar\omega - \frac{\lambda^2\hbar}{8m^2\omega^3}.$$

The ground state to first order will be

$$\left|\psi_{000}\right\rangle = \left|000\right\rangle + \sum_{mnp\neq 000}\left|000\right\rangle\frac{\left\langle mnp\right|W\left|000\right\rangle}{\varepsilon_{000} - \varepsilon_{mnp}} = \left|000\right\rangle + \left|110\right\rangle\frac{\lambda\hbar}{2m\omega(-2\omega)} = \left|000\right\rangle - \frac{\lambda\hbar}{4m\omega^2}\left|110\right\rangle.$$

There are three first excited states, namely, $\left|100\right\rangle$, $\left|010\right\rangle$, $\left|001\right\rangle$. We work out W acting on each of these to yield

$$W\left|100\right\rangle = \frac{\lambda\hbar}{2m\omega}\left(a_x + a_x^\dagger\right)\left(a_y + a_y^\dagger\right)\left|100\right\rangle = \frac{\lambda\hbar}{2m\omega}\left(a_x + a_x^\dagger\right)\left|110\right\rangle = \frac{\lambda\hbar}{2m\omega}\left(\left|010\right\rangle + \sqrt{2}\left|210\right\rangle\right),$$

$$W\left|010\right\rangle = \frac{\lambda\hbar}{2m\omega}\left(a_x + a_x^\dagger\right)\left(a_y + a_y^\dagger\right)\left|010\right\rangle = \frac{\lambda\hbar}{2m\omega}\left(a_x + a_x^\dagger\right)\left(\left|000\right\rangle + \sqrt{2}\left|020\right\rangle\right)$$

$$= \frac{\lambda\hbar}{2m\omega}\left(\left|100\right\rangle + \sqrt{2}\left|120\right\rangle\right),$$

$$W\left|001\right\rangle = \frac{\lambda\hbar}{2m\omega}\left(a_x + a_x^\dagger\right)\left(a_y + a_y^\dagger\right)\left|001\right\rangle = \frac{\lambda\hbar}{2m\omega}\left(a_x + a_x^\dagger\right)\left|011\right\rangle = \frac{\lambda\hbar}{2m\omega}\left|111\right\rangle.$$

There are only two nonzero matrix elements, $\left\langle 010\right|W\left|100\right\rangle$ and $\left\langle 100\right|W\left|010\right\rangle$, so if we list the states in the order $\left\{\left|100\right\rangle, \left|010\right\rangle, \left|001\right\rangle\right\}$, the $\tilde{W}$ matrix will be

$$\tilde{W} = \frac{\lambda\hbar}{2m\omega}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

This matrix is clearly block diagonal, and we see that the third state $\left|001\right\rangle$ doesn't mix at all. The other two states are $\frac{1}{\sqrt{2}}\left(\left|100\right\rangle \pm \left|010\right\rangle\right)$, so in summary we have

$$E_\pm = \frac{3}{2}\hbar\omega \pm \frac{\lambda\hbar}{2m\omega}, \quad \left|\psi_\pm\right\rangle = \frac{1}{\sqrt{2}}\left(\left|100\right\rangle \pm \left|010\right\rangle\right),$$

$$E_0 = \frac{3}{2}\hbar\omega, \qquad \left|\psi_0\right\rangle = \left|001\right\rangle.$$

3. [20] A particle of mass *m* in 3D in the potential $V(r) = -\frac{2}{3}\beta r^{-3/2}$. Using the variational principle with trial wave function $\psi(r) = e^{-\lambda r/2}$, estimate the energy of the ground state.

We need to calculate $\langle\psi|\psi\rangle$, $\langle\psi|\mathbf{P}^2|\psi\rangle$ and $\langle\psi|V(r)|\psi\rangle$. For the kinetic term it is often easier to calculate $\langle\psi|\mathbf{P}^2|\psi\rangle = \|\mathbf{P}|\psi\rangle\|^2$. The quantities are

$$\langle\psi|\psi\rangle = \int|\psi|^2 d^3\mathbf{r} = \int\left(e^{-\lambda r/2}\right)^2 d^3\mathbf{r} = \int_0^\infty e^{-\lambda r} r^2 dr \int d\Omega = 4\pi\frac{2!}{\lambda^3} = \frac{8\pi}{\lambda^3},$$

$$\left\langle\mathbf{P}^2\right\rangle = \|\mathbf{P}|\psi\rangle\|^2 = \int\left|-i\hbar\nabla e^{-\lambda r/2}\right|^2 d^3\mathbf{r} = \hbar^2\tfrac{1}{4}\lambda^2\int\left(e^{-\lambda r/2}\right)^2 d^3\mathbf{r} = \frac{2\pi\hbar^2}{\lambda},$$

$$\left\langle V(r)\right\rangle = \int V(r)\left|e^{-\lambda r/2}\right|^2 d^3\mathbf{r} = -\frac{2}{3}\beta\int_0^\infty e^{-\lambda r}r^2 r^{-3/2}dr\int d\Omega = -\frac{8}{3}\pi\beta\int_0^\infty r^{1/2}e^{-\lambda r}dr = -6\pi\beta\frac{\Gamma\left(\frac{3}{2}\right)}{\lambda^{3/2}}$$
$$= -\frac{4\pi\beta\sqrt{\pi}}{3\lambda^{3/2}}.$$

We now put this all together into a formula for the energy, which is

$$E(\lambda) = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{1}{\langle\psi|\psi\rangle}\left(\frac{1}{2m}\left\langle\mathbf{P}^2\right\rangle + \left\langle V(r)\right\rangle\right) = \frac{\lambda^3}{8\pi}\left(\frac{2\pi\hbar^2}{2m\lambda} - \frac{4\pi\beta\sqrt{\pi}}{3\lambda^{3/2}}\right) = \frac{\hbar^2\lambda^2}{8m} - \frac{\beta\sqrt{\pi}\lambda^{3/2}}{6}.$$

We now want to find the minimum of this potential, which we take by setting the derivative to zero to yield

$$0 = \frac{d}{d\lambda}\left(\frac{\hbar^2\lambda^2}{8m} - \frac{\beta\sqrt{\pi}\lambda^{3/2}}{6}\right) = \frac{\hbar^2\lambda}{4m} - \frac{\beta\sqrt{\pi}\lambda^{1/2}}{4},$$

$$\sqrt{\lambda} = \frac{\beta m\sqrt{\pi}}{\hbar^2},$$

$$\lambda = \frac{\pi\beta^2 m^2}{\hbar^4}.$$

We now substitute this back into the formula for the energy, which yields

$$E_0 \approx \frac{\hbar^2}{8m}\left(\frac{\pi\beta^2 m^2}{\hbar^4}\right)^2 - \frac{\beta\sqrt{\pi}}{6}\left(\frac{\pi\beta^2 m^2}{\hbar^4}\right)^{3/2} = \frac{\pi^2\beta^4 m^3}{\hbar^6}\left(\frac{1}{8} - \frac{1}{6}\right) = -\frac{\pi^2\beta^4 m^3}{24\hbar^6}.$$

4. [20] The hydrogen nucleus is normally assumed to be a point charge, leading to an electrostatic potential $U(r)=k_e e/r$. Suppose that the effect of the finite size of the nucleus is that this is modified to $U(r)=\frac{k_e e}{r}\left(1-e^{-r/R}\right)$, where the scale of the nucleus *R* is much smaller than the radius of the atom *a*. Find an approximate formula for the energy shift ε', and argue that it vanishes except for s-wave state (l = 0). Find a formula for the shift in energy for the 1s state of hydrogen, with unperturbed wave function $\psi(r)=e^{-r/a}\big/\sqrt{\pi a^3}$.

The potential is the electrostatic potential times the electron charge, which is –*e*. Adding the kinetic term yields a Hamiltonian

$$H=\frac{\mathbf{P}^2}{2\mu}-eU(r)=\frac{\mathbf{P}^2}{2\mu}-\frac{k_e e^2}{r}\left(1-e^{-r/R}\right).$$

We then split this into two terms, an unperturbed Hamiltonian $H_0=\mathbf{P}^2/2\mu-k_e e^2/r$, and a perturbation $W=k_e e^2 e^{-r/R}/r$. This causes a first-order shift in the energy given by

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

The charge distribution falls quickly to zero on a scale of about *R*, and on this scale, the atomic wave functions are almost constant. We therefore approximate $\psi_{nlm}(\mathbf{r})\approx\psi_{nlm}(0)$, so we have

$$\begin{aligned}\varepsilon'&=\langle nlm|W|nlm\rangle=k_e e^2\left|\psi_{nlm}(0)\right|^2\int r^{-1}e^{-r/R}d^3\mathbf{r}=k_e e^2\left|\psi_{nlm}(0)\right|^2\int d\Omega\int_0^\infty r^{-1}e^{-r/R}r^2dr\\&=4\pi k_e e^2\left|\psi_{nlm}(0)\right|^2\int_0^\infty e^{-r/R}rdr=4\pi k_e e^2\left|\psi_{nlm}(0)\right|^2R^2.\end{aligned}$$

We note that the wave function $\psi_{nlm}(0)$ vanishes except for $l=0$, so the contribution vanishes in every other case. We could further simplify this expression using $Y_0^0=1\big/\sqrt{4\pi}$ to simplify the expression to $\varepsilon'_{n00}=k_e e^2R^2R_{n0}^2(0)$. Applying the formula to the 1s state of hydrogen, we have

$$\varepsilon'_{100}=4\pi k_e e^2R^2\frac{1}{\pi a^3}=\frac{4k_e e^2R^2}{a^3}.$$

5. [20] A particle of mass μ and wave number *k* scatters from a potential $V = \beta r^{-3/2}$, where β is small. Find the differential cross-section in the first Born approximation, and the total cross-section for scattering by angles $\theta > \frac{1}{2}\pi$. Hint: when doing the Fourier transform, I recommend doing the radial integral last.

We need to find the Fourier transform of the potential. Because the potential is spherically symmetric, the direction of **K** can't matter, and hence we can treat it as if it is in the *z*-direction, so that $\mathbf{K}\cdot\mathbf{r} = Kr\cos\theta$. We work in spherical coordinates, and we can, in fact, do the integrals in either order, so we have

$$\int d^3\mathbf{r}V(\mathbf{r})e^{-i\mathbf{K}\cdot\mathbf{r}} = \beta\int_0^{2\pi}d\phi\int_0^\infty r^2 r^{-3/2}dr\int_{-1}^1 e^{-iKr\cos\theta}d(\cos\theta) = 2\pi\beta\int_0^\infty \sqrt{r}dr\frac{1}{-iKr}e^{-iKr\cos\theta}\Big|_{-1}^1$$
$$= \frac{2\pi\beta i}{K}\int_0^\infty\left(e^{-iKr}-e^{iKr}\right)r^{-1/2}dr = \frac{2\pi\beta i}{K}\Gamma\left(\tfrac{1}{2}\right)\left(\frac{1}{\sqrt{iK}}-\frac{1}{\sqrt{-iK}}\right)$$
$$= \frac{2\pi\sqrt{\pi}\beta i}{K^{3/2}}\left[\frac{1}{\sqrt{2}}(1-i)-\frac{1}{\sqrt{2}}(1+i)\right] = \frac{2\pi\sqrt{\pi}\beta i}{K^{3/2}}\left(-\sqrt{2}i\right) = \frac{2\pi\sqrt{2\pi}\beta}{K^{3/2}}.$$

We now substitute this into the equation for the Born approximation, which yields

$$\frac{d\sigma}{d\Omega} = \frac{\mu^2}{4\pi^2\hbar^4}\left|\int d^3\mathbf{r}V(\mathbf{r})e^{-i\mathbf{K}\cdot\mathbf{r}}\right|^2 = \frac{\mu^2}{4\pi^2\hbar^4}\left(\frac{2\pi\sqrt{2\pi}\beta}{K^{3/2}}\right)^2 = \frac{\mu^2 8\pi^3\beta^2}{4\pi^2\hbar^4K^3} = \frac{2\pi\mu^2\beta^2}{\hbar^4\left[2k^2(1-\cos\theta)\right]^{3/2}}.$$

The total cross section is then obtained by integrating over angles, but we want to only include angles in the range $\frac{1}{2}\pi < \theta < \pi$, which corresponds to $-1 < \cos\theta < 0$, so we have

$$\sigma = \int\frac{d\sigma}{d\Omega}d\Omega = \frac{2\pi\mu^2\beta^2}{\hbar^4\left(2k^2\right)^{3/2}}\int_0^{2\pi}d\phi\int_{-1}^0\frac{d(\cos\theta)}{(1-\cos\theta)^{3/2}} = \frac{4\pi^2\mu^2\beta^2}{\hbar^4 2^{3/2}k^3}2(1-\cos\theta)^{-1/2}\Big|_{-1}^0$$
$$= \frac{2\sqrt{2}\pi^2\mu^2\beta^2}{\hbar^4k^3}\left(\frac{1}{1}-\frac{1}{\sqrt{2}}\right) = \frac{2\left(\sqrt{2}-1\right)\pi^2\mu^2\beta^2}{\hbar^4k^3}.$$

Had we integrated over all angles, the integral would have diverged in the forward direction, due to the long-range nature of the integral.

Possibly Helpful Formulas:

Born Approximation

$$\frac{d\sigma}{d\Omega} = \frac{\mu^2}{4\pi^2\hbar^4}\left|\int d^3\mathbf{r}\, V(\mathbf{r})\, e^{-i\mathbf{K}\cdot\mathbf{r}}\right|^2$$

$$\mathbf{K}^2 = 2k^2(1-\cos\theta)$$

1D Harmonic Oscillator

$$X = \sqrt{\frac{\hbar}{2m\omega}}\left(a + a^\dagger\right)$$

$$a|n\rangle = \sqrt{n}\,|n-1\rangle$$

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

Spherical Coordinates

$$\nabla\psi = \hat{\mathbf{r}}\frac{\partial\psi}{\partial r} + \hat{\boldsymbol{\theta}}\frac{1}{r}\frac{\partial\psi}{\partial\theta} + \hat{\phi}\frac{1}{r\sin\theta}\frac{\partial\psi}{\partial\phi}$$

$$\nabla^2\psi = \frac{\partial^2\psi}{\partial r^2} + \frac{2}{r}\frac{\partial\psi}{\partial r} + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}$$

Math

$$\sqrt{\pm i} = \frac{1}{\sqrt{\mp i}} = \frac{1}{\sqrt{2}}(1\pm i)$$

Possibly Helpful Integrals:

$$\int_0^\infty x^n e^{-Ax}dx = \begin{cases} n!/A^{n+1} & n \text{ integer,} \\ \Gamma(n+1)/A^{n+1} & \text{all } n. \end{cases}$$

$$\int_0^\pi e^{-iA\cos\theta}\sin\theta\, d\theta = 2\sin(A)/A,$$

$$\int_0^\infty x^n \sin(Bx)\, dx = \frac{\Gamma(n+1)}{B^{n+1}}\sin\left[\tfrac{1}{2}\pi(n+1)\right],$$

$$\Gamma\left(\tfrac{1}{2}\right) = \sqrt{\pi},$$

$$\Gamma\left(\tfrac{3}{2}\right) = \tfrac{1}{2}\sqrt{\pi},$$

$$\Gamma\left(\tfrac{5}{2}\right) = \tfrac{3}{4}\sqrt{\pi}.$$