Physics 742 – Graduate Quantum Mechanics 2

Solutions to First Exam, Spring 2019

Please note that some possibly helpful formulas are listed below or on the handout. Each question is worth twenty points.

1. A particle of mass *m* in one dimension is in the potential $V(x)=\alpha\sqrt{|x|}$. Using the WKB method, estimate the energy of the *n*'th eigenstate. *Hint*: I found it useful to define $x=y^2$ and $z=E-\alpha y$.

We first need to find the turning points, the points where $E=V(x)=\alpha\sqrt{|x|}$. It is pretty trivial to rewrite this as $|x|=E^2/\alpha^2$, with solutions $x=\pm E^2/\alpha^2$. We therefore have

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

We now make two substitutions: first, let $x=y^2$, and then let $z=E-\alpha y$. The latter can be inverted to give $y=(E-z)/\alpha$. We then have

$$\pi\hbar\left(n+\tfrac{1}{2}\right)=2\int_0^{E/\alpha}2y\,dy\sqrt{2m(E-\alpha y)}=\frac{4}{\alpha^2}\int_E^0(E-z)\,d(E-z)\sqrt{2mz}=\frac{4\sqrt{2m}}{\alpha^2}\int_0^E\left(Ez^{1/2}-z^{3/2}\right)dz$$
$$=\frac{4\sqrt{2m}}{\alpha^2}\left(\tfrac{2}{3}Ez^{3/2}-\tfrac{2}{5}z^{5/2}\right)\Big|_0^E=\frac{4\sqrt{2m}}{\alpha^2}E^{5/2}\left(\tfrac{2}{3}-\tfrac{2}{5}\right)=\frac{16\sqrt{2m}}{15\alpha^2}E^{5/2}.$$

It is now straightforward to solve this for *E*, so we have

$$E=\left[\frac{15\pi\alpha^2\hbar\left(n+\frac{1}{2}\right)}{16\sqrt{2m}}\right]^{2/5}=\frac{\alpha^{4/5}\hbar^{2/5}\pi^{2/5}}{m^{1/5}}\left[\frac{15}{16\sqrt{2}}\left(n+\tfrac{1}{2}\right)\right]^{2/5}.$$

It is worth noting the similarity of functional form of this expression and the form for the next problem. If you substitute *n* = 0 in this formula, the final factor from this equation works out to 0.6429, and the next equation yields 0.625.

Possibly Helpful Integrals

$$\int_0^\infty x^n e^{-Ax}dx=\begin{cases}n!/A^{n+1} & n\text{ integer,}\\ \Gamma(n+1)/A^{n+1} & \text{all } n.\end{cases}\qquad \int_{-\infty}^{\infty}e^{-Ax^2/2+Bx}dx=\sqrt{\frac{2\pi}{A}}e^{B^2/2A},$$

$$\Gamma\left(\tfrac{1}{2}\right)=\sqrt{\pi},\quad \Gamma\left(\tfrac{3}{2}\right)=\tfrac{1}{2}\sqrt{\pi},\quad \Gamma\left(\tfrac{5}{2}\right)=\tfrac{3}{4}\sqrt{\pi}.\qquad \int_{-\infty}^{\infty}xe^{-Ax^2/2+Bx}dx=\frac{B}{A}\sqrt{\frac{2\pi}{A}}e^{B^2/2A}.$$

$$\int_0^{2\pi}\sin^2\phi\,d\phi=\int_0^{2\pi}\cos^2\phi\,d\phi=\pi,\quad \int_0^{2\pi}\sin^4\phi\,d\phi=\int_0^{2\pi}\cos^4\phi\,d\phi=\tfrac{3}{4}\pi,\quad \int_0^{2\pi}\sin^2\phi\cos^2\phi\,d\phi=\tfrac{1}{4}\pi.$$

2. A particle of mass *m* in one dimension is in the potential $V(x)=\alpha\sqrt{|x|}$. Using the variational principle with trial wave function $\psi(x)=e^{-\lambda|x|/2}$, estimate the energy of the ground state. I recommend using $\langle\psi|P^2|\psi\rangle=|P|\psi\rangle|^2$ when estimating the kinetic term.

We need to calculate $\langle\psi|\psi\rangle$, $\langle\psi|P^2|\psi\rangle$, and $\langle\psi|V(x)|\psi\rangle$. We have

$$\langle\psi|\psi\rangle=\int_{-\infty}^{\infty}|\psi|^2\,dx=\int_{-\infty}^{\infty}e^{-\lambda|x|}dx=2\int_0^\infty e^{-\lambda x}dx=\frac{2\cdot 1!}{\lambda}=\frac{2}{\lambda},$$

$$\langle\psi|P^2|\psi\rangle=|P|\psi\rangle|^2=\int_{-\infty}^{\infty}\left|-i\hbar\frac{d}{dx}e^{-\lambda|x|/2}\right|^2dx=2\hbar^2\int_0^\infty\left|\frac{d}{dx}e^{-\lambda x/2}\right|^2dx=2\hbar^2\int_0^\infty\left|-\tfrac{1}{2}\lambda e^{-\lambda x}\right|^2dx$$

$$=\frac{\lambda^2\hbar^2}{2}\int_0^\infty e^{-\lambda x}dx=\frac{\lambda^2\hbar^2}{2\lambda}=\frac{\lambda\hbar^2}{2},$$

$$\langle\psi|V(x)|\psi\rangle=\int_{-\infty}^{\infty}\left|e^{-\lambda|x|/2}\right|^2\alpha\sqrt{|x|}dx=2\alpha\int_0^\infty e^{-\lambda x}x^{1/2}dx=\frac{2\alpha}{\lambda^{3/2}}\Gamma\left(\tfrac{3}{2}\right)=\alpha\lambda^{-3/2}\sqrt{\pi}.$$

The normalized expectation value of the energy, therefore, would be

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

We now wish to minimize this with respect to λ, which we do by taking the derivative.

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

$$\lambda^{5/2}=\frac{m\alpha\sqrt{\pi}}{\hbar^2},$$

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

We now substitute this back in to estimate the ground state energy:

$$E_{\min}=\frac{\hbar^2}{8m}\left(\frac{m\alpha\sqrt{\pi}}{\hbar^2}\right)^{4/5}+\frac{\alpha\sqrt{\pi}}{2}\left(\frac{m\alpha\sqrt{\pi}}{\hbar^2}\right)^{-1/5}=\frac{\hbar^{2/5}\alpha^{4/5}\pi^{2/5}}{m^{1/5}}\left(\frac{1}{8}+\frac{1}{2}\right)=\frac{5\hbar^{2/5}\alpha^{4/5}\pi^{2/5}}{8m^{1/5}}.$$

3. A particle of mass *m* in two dimensions is in the potential $V(x)=\frac{1}{2}m\omega^2\left(X^2+Y^2\right)+\delta X^2Y^2$, where δ is small. Name and find the energies of the eigenstates of the unperturbed Hamiltonian in the limit $\delta=0$. Find the ground state eigenstate to first order in δ, and its energy to second order in δ.

To find the ground state eigenstate we need to find $W|00\rangle$, which is

$$W|00\rangle=\delta X^2Y^2|00\rangle=\delta\left(\frac{\hbar}{2m\omega}\right)^2\left(a_x+a_x^\dagger\right)^2\left(a_y+a_y^\dagger\right)^2|00\rangle=\frac{\delta\hbar^2}{4m^2\omega^2}\left(a_x+a_x^\dagger\right)^2\left(a_y+a_y^\dagger\right)|01\rangle$$
$$=\frac{\delta\hbar^2}{4m^2\omega^2}\left(a_x+a_x^\dagger\right)^2\left(|00\rangle+\sqrt{2}|02\rangle\right)=\frac{\delta\hbar^2}{4m^2\omega^2}\left(a_x+a_x^\dagger\right)\left(|10\rangle+\sqrt{2}|12\rangle\right)$$
$$=\frac{\delta\hbar^2}{4m^2\omega^2}\left(|00\rangle+\sqrt{2}|20\rangle+\sqrt{2}|02\rangle+2|22\rangle\right).$$

The ground state eigenstate, to first order in δ, is

$$|\psi_{00}\rangle=|00\rangle+\sum_{nm\neq00}|nm\rangle\frac{\langle nm|W|00\rangle}{\varepsilon_{00}-\varepsilon_{nm}}=|00\rangle+|20\rangle\frac{\langle20|W|00\rangle}{\varepsilon_{00}-\varepsilon_{20}}+|02\rangle\frac{\langle02|W|00\rangle}{\varepsilon_{00}-\varepsilon_{02}}+|22\rangle\frac{\langle22|W|00\rangle}{\varepsilon_{00}-\varepsilon_{20}}$$
$$=|00\rangle+\frac{\delta\hbar^2}{4m^2\omega^2}\left(\frac{\sqrt{2}|20\rangle}{\hbar\omega-3\hbar\omega}+\frac{\sqrt{2}|02\rangle}{\hbar\omega-3\hbar\omega}+\frac{2|22\rangle}{\hbar\omega-5\hbar\omega}\right)$$
$$=|00\rangle-\frac{\delta\hbar}{8m^2\omega^3}\left(\sqrt{2}|20\rangle+\sqrt{2}|02\rangle+|22\rangle\right).$$

The ground state energy is given by

$$E_{00}=\varepsilon_{00}+\langle00|W|00\rangle+\sum_{nm\neq00}\frac{\left|\langle nm|W|00\rangle\right|^2}{\varepsilon_{00}-\varepsilon_{nm}}$$
$$=\hbar\omega+\frac{\delta\hbar^2}{4m^2\omega^2}+\frac{\left|\langle20|W|00\rangle\right|^2}{\varepsilon_{00}-\varepsilon_{20}}+\frac{\left|\langle02|W|00\rangle\right|^2}{\varepsilon_{00}-\varepsilon_{02}}+\frac{\left|\langle22|W|00\rangle\right|^2}{\varepsilon_{00}-\varepsilon_{22}}$$
$$=\hbar\omega+\frac{\delta\hbar^2}{4m^2\omega^2}+\left(\frac{\delta\hbar^2}{4m^2\omega^2}\right)^2\left[\frac{\left(\sqrt{2}\right)^2}{\hbar\omega-3\hbar\omega}+\frac{\left(\sqrt{2}\right)^2}{\hbar\omega-3\hbar\omega}+\frac{2^2}{\hbar\omega-5\hbar\omega}\right]$$
$$=\hbar\omega+\frac{\delta\hbar^2}{4m^2\omega^2}+\frac{\delta^2\hbar^3}{16m^4\omega^5}\left(-1-1-1\right)=\hbar\omega+\frac{\delta\hbar^2}{4m^2\omega^2}-\frac{3\delta^2\hbar^3}{16m^4\omega^5}.$$

4. An electron is in a three-dimensional harmonic oscillator with Coulomb potential $V_c(r) = \frac{1}{2}m\omega^2 r^2$.

(a) Write the spin-orbit coupling in terms of $\mathbf{L}^2$, $\mathbf{S}^2$, and $\mathbf{J}^2$, where $\mathbf{J} = \mathbf{L} + \mathbf{S}$.

We start by using the standard trick of writing

$$\mathbf{L}\cdot\mathbf{S} = \tfrac{1}{2}(\mathbf{L}+\mathbf{S})^2 - \tfrac{1}{2}\mathbf{L}^2 - \tfrac{1}{2}\mathbf{S}^2 = \tfrac{1}{2}\mathbf{J}^2 - \tfrac{1}{2}\mathbf{L}^2 - \tfrac{1}{2}\mathbf{S}^2$$

Substituting this in, together with the given Coulomb potential, we have

$$W_{\text{SO}} = \frac{g}{4m^2c^2}\frac{1}{r}\frac{dV_c(r)}{dr}\mathbf{L}\cdot\mathbf{S} = \frac{g}{8m^2c^2}\frac{1}{r}\frac{d}{dr}\left(\frac{1}{2}m\omega^2 r^2\right)\left(\mathbf{J}^2 - \mathbf{L}^2 - \mathbf{S}^2\right) = \frac{gm\omega^2 r}{8m^2c^2 r}\left(\mathbf{J}^2 - \mathbf{L}^2 - \mathbf{S}^2\right).$$

(b) For $l = 0$, what are the eigenvalues or possible eigenvalues of $\mathbf{L}^2$, $\mathbf{S}^2$, and $\mathbf{J}^2$? Argue that for states with $l = 0$, the spin-orbit coupling causes no shift in energy.

Electrons have spin ½, and j runs from $|l-s|$ to $|l+s|$. In the case of $l = 0$, the only possibility is $j = \frac{1}{2} = s$, and therefore $\mathbf{J}^2 = \mathbf{S}^2 = \hbar^2\left(\frac{1}{4}+\frac{1}{2}\right) = \frac{3}{4}\hbar^2$, while $\mathbf{L}^2 = \hbar^2(0+0) = 0$. Hence

$$W_{\text{SO}}\left|l=0, s=\tfrac{1}{2}, j, m_j\right\rangle = \frac{g\omega^2}{8mc^2}\left[\tfrac{3}{4}\hbar^2 - 0 - \tfrac{3}{4}\hbar^2\right]\left|l=0, s=\tfrac{1}{2}, j, m_j\right\rangle = 0.$$

Hence there is no shift in the energy.

(c) For $l = 1$, what are the eigenvalues or possible eigenvalues of $\mathbf{L}^2$, $\mathbf{S}^2$, and $\mathbf{J}^2$? Find the corresponding shift in energies.

We still have $\mathbf{S}^2 = \frac{3}{4}\hbar^2$, but now j can take on the values $j = |l-s| = \left|1-\frac{1}{2}\right| = \frac{1}{2}$ or $j = l+s = 1+\frac{1}{2} = \frac{3}{2}$, and therefore we can have either $\mathbf{J}^2 = \frac{3}{4}\hbar^2$ or $\mathbf{J}^2 = \left(\frac{9}{4}+\frac{3}{2}\right)\hbar^2 = \frac{15}{4}\hbar^2$. We also now have $\mathbf{L}^2 = (1+1)\hbar^2 = 2\hbar^2$ We therefore have two possibilities:

$$W_{\text{SO}}\left|l=1, s=\tfrac{1}{2}, j=\tfrac{1}{2}, m_j\right\rangle = \frac{g\omega^2}{8mc^2}\left[\tfrac{3}{4}\hbar^2 - 2\hbar^2 - \tfrac{3}{4}\hbar^2\right]\left|l=0, s=\tfrac{1}{2}, j, m_j\right\rangle = -\frac{g\omega^2\hbar^2}{4mc^2},$$

$$W_{\text{SO}}\left|l=1, s=\tfrac{1}{2}, j=\tfrac{3}{2}, m_j\right\rangle = \frac{g\omega^2}{8mc^2}\left[\tfrac{15}{4}\hbar^2 - 2\hbar^2 - \tfrac{3}{4}\hbar^2\right]\left|l=0, s=\tfrac{1}{2}, j, m_j\right\rangle = \frac{g\omega^2\hbar^2}{8mc^2}.$$

5. **A particle of mass μ and wave number *k* moving in the +*z* direction scatters from a potential $V = V_0 xy e^{-\alpha \mathbf{r}^2/2}$, where V_0 is small. Find the differential and total cross-section in the first Born approximation. For the total cross-section, you may leave one integral uncompleted.**

We must first find the Fourier transform. In this case, this is most easily done in Cartesian coordinates, so we have

$$
\begin{aligned}
\int V(\mathbf{r}) e^{-i\mathbf{K}\cdot\mathbf{r}} d^3\mathbf{r} &= \int V_0 xy e^{-\alpha \mathbf{r}^2/2} e^{-i\mathbf{K}\cdot\mathbf{r}} d^3\mathbf{r} = V_0 \int_{-\infty}^{\infty} x e^{-iK_x x - \alpha x^2/2} dx \int_{-\infty}^{\infty} y e^{-iK_y y - \alpha y^2/2} dy \int_{-\infty}^{\infty} e^{-iK_z z - \alpha z^2/2} dz \\
&= V_0 \left(\frac{-iK_x}{\alpha} \sqrt{\frac{2\pi}{\alpha}} e^{-K_x^2/2\alpha} \right) \left(\frac{-iK_y}{\alpha} \sqrt{\frac{2\pi}{\alpha}} e^{-K_y^2/2\alpha} \right) \left(\sqrt{\frac{2\pi}{\alpha}} e^{-K_z^2/2\alpha} \right) \\
&= -(2\pi)^{3/2} \alpha^{-7/2} V_0 K_x K_y e^{-\mathbf{K}^2/2\alpha} .
\end{aligned}
$$

We now substitute this into the formula for differential cross-section to yield

$$
\frac{d\sigma}{d\Omega} = \frac{\mu^2}{4\pi^2\hbar^4} \left| \int d^3\mathbf{r} V(\mathbf{r}) e^{-i\mathbf{K}\cdot\mathbf{r}} \right|^2 = \frac{\mu^2 K_x^2 K_y^2 V_0^2 (2\pi)^3}{4\pi^2 \hbar^4 \alpha^7} e^{-\mathbf{K}^2/\alpha}
$$

We now recall that $\mathbf{K} = \mathbf{k}' - \mathbf{k}$. The initial momentum is $\mathbf{k} = k\hat{\mathbf{z}}$, and the final is $\mathbf{k}' = k\hat{\mathbf{r}}$, so

$$
\mathbf{K} = \mathbf{k}' - \mathbf{k} = k\hat{\mathbf{r}} - k\hat{\mathbf{z}} = k(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta - 1)
$$

We also can use the formulal (or rederive it) $\mathbf{K}^2 = 2k^2(1-\cos\theta)$. We therefore have

$$
\frac{d\sigma}{d\Omega} = \frac{\mu^2}{4\pi^2\hbar^4} \left| \int d^3\mathbf{r} V(\mathbf{r}) e^{-i\mathbf{K}\cdot\mathbf{r}} \right|^2 = \frac{2\pi\mu^2 k^4}{\hbar^4 \alpha^7} V_0^2 \sin^4\theta \cos^2\phi \sin^2\phi \, e^{-2k^2(1-\cos\theta)/\alpha} .
$$

We now simply integrate this over solid angle, so we have

$$
\begin{aligned}
\sigma &= \int \frac{d\sigma}{d\Omega} d\Omega = \frac{2\pi\mu^2 k^4}{\hbar^4 \alpha^7} \int_{-1}^{1} \sin^4\theta e^{-2k^2(1-\cos\theta)/\alpha} d(\cos\theta) \int_0^{2\pi} \cos^2\phi \sin^2\phi \, d\phi \\
&= \frac{\pi^2 \mu^2 k^4}{2\hbar^4 \alpha^7} \int_{-1}^{1} \left(1 - \cos^2\theta\right)^2 e^{-2k^2(1-\cos\theta)/\alpha} d(\cos\theta).
\end{aligned}
$$

There is nothing inherently difficult about the final integral, but the result will be annoyingly complicated, so we'll just leave this last integral undone.

Possibly Helpful Formulas

Spin-Orbit Coupling	**Born Approximation**	**1D Harmonic Oscillator**
$W_{SO} = \frac{g}{4m^2c^2} \frac{1}{r} \frac{dV_c(r)}{dr} \mathbf{L}\cdot\mathbf{S}$	$\frac{d\sigma}{d\Omega} = \frac{\mu^2}{4\pi^2\hbar^4} \left\lvert \int d^3\mathbf{r} V(\mathbf{r}) e^{-i\mathbf{K}\cdot\mathbf{r}} \right\rvert^2$	$X = \sqrt{\frac{\hbar}{2m\omega}} \left(a + a^\dagger\right)$
	$\mathbf{K}^2 = 2k^2(1-\cos\theta)$	$a\lvert n\rangle = \sqrt{n}\lvert n-1\rangle$
		$a^\dagger\lvert n\rangle = \sqrt{n+1}\lvert n+1\rangle$