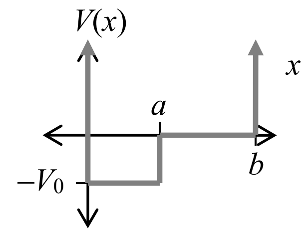
Quantum Mechanics
Solutions to Graduate Exam

Summer, 2021

Each problem is worth 25 points. The points for individual parts are marked in square brackets. **To ensure full credit, show your work.** Do any four (4) of the following five (5) problems. If you attempt all 5 problems you must clearly state which 4 problems you want to have graded.

1. A particle of mass *m* has energy eigenvalue *E* = 0 in the 1D potential sketched below,

$$V(x)=\begin{cases}-V_0 & \text{if } 0<x<a,\\ 0 & \text{if } a<x<b,\\ \infty & \text{otherwise.}\end{cases}$$



Find an expression for *b* in terms of *a*, V_0 and *m*.

We need to solve Schrodinger's equation in each of the two regions and match the boundary conditions as appropriate at each boundary. In the region $0<x<a$, the potential is $-V_0$, and using the fact that the energy is $E = 0$, Schrodinger's equation is $0=-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}-V_0\psi$. Thus ψ must be proportional to its negative second derivative, which will work for functions like $\psi(x)=N\cos(kx)$ or $\psi(x)=N\sin(kx)$. Because we want the wave function to vanish at the boundary $x = 0$ where the potential becomes infinite, we choose sine. The value of k is given by the expression $V_0=\hbar^2k^2/2m$, which can be solved for k to give $k=\sqrt{2mV_0}/\hbar$.

In the regions $a<x<b$, Schrodinger's equation becomes even simpler, so that $\frac{d^2\psi}{dx^2}=0$. The only functions that have vanishing second derivative are linear functions. But it must also vanish at $x = b$, so we have

$$\psi(x)=\begin{cases}N\sin(kx) & 0<x<a,\\ \alpha(b-x) & a<x<b.\end{cases}$$

At the shared boundary $x = a$, the functions must match and their derivatives match, so we have

$$N\sin(ka)=\alpha(b-a) \quad\text{and}\quad Nk\cos(ka)=-\alpha.$$

Taking the ratio of these two equations, we have

$$k^{-1}\tan(ka)=a-b.$$

Solving for b, we find

$$b=a-\frac{1}{k}\tan(ka)=a-\frac{\hbar}{\sqrt{2mV_0}}\tan\left(\frac{a\sqrt{2mV_0}}{\hbar}\right).$$

2. **An electron is in a magnetic field pointing in the z-direction, $\mathbf{B} = B\hat{\mathbf{z}}$. The Hamiltonian is given by $H = -\gamma \mathbf{B}\cdot\mathbf{S}$. Several helpful formulas appear at the end of this problem.**
(a) [2] What are the eigenvalues and eigenvectors for the energy?

The eigenstates are the eigenstates of the diagonal matrix σ_z, which are trivial, and the eigenvalues are simply $-\frac{1}{2}\gamma B\hbar$ times ± 1, so we have

$$\left|+\right\rangle = \begin{pmatrix}1\\0\end{pmatrix}, \quad \left|-\right\rangle = \begin{pmatrix}0\\1\end{pmatrix}, \quad E_\pm = \mp\tfrac{1}{2}\gamma\hbar B.$$

(b) [6] If the system at $t = 0$ is in the state $\left|\Psi(0)\right\rangle = \begin{pmatrix}\cos\theta\\ \sin\theta\end{pmatrix}$, what is the state at time t, $\left|\Psi(t)\right\rangle$?

It is obvious that the original state can be written as $\left|\Psi(0)\right\rangle = \cos\theta\left|+\right\rangle + \sin\theta\left|-\right\rangle$. The time evolution simply causes each eigenstate to be multiplied by a phase $\exp\left(-iE_\pm t/\hbar\right) = e^{\pm i\gamma Bt/2}$. Therefore, at time t the state will be

$$\left|\Psi(t)\right\rangle = \cos\theta e^{i\gamma Bt/2}\left|+\right\rangle + \sin\theta e^{-i\gamma Bt/2}\left|-\right\rangle = \begin{pmatrix}\cos\theta e^{i\gamma Bt/2}\\ \sin\theta e^{-i\gamma Bt/2}\end{pmatrix}.$$

(c) [6] Calculate the expectation value of the three spin operators $\left\langle S_x\right\rangle$, $\left\langle S_y\right\rangle$, and $\left\langle S_z\right\rangle$ at time t.

The expectation values can be calculated simply by writing out explicitly $\left\langle S_i\right\rangle = \frac{1}{2}\hbar\left\langle\Psi\right|\sigma_i\left|\Psi\right\rangle$, which works out to

$$\left\langle S_x\right\rangle = \frac{1}{2}\hbar\begin{pmatrix}e^{-i\gamma Bt/2}\cos\theta & e^{i\gamma Bt/2}\sin\theta\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}e^{i\gamma Bt/2}\cos\theta\\ e^{-i\gamma Bt/2}\sin\theta\end{pmatrix} = \frac{1}{2}\hbar\sin\theta\cos\theta\left(e^{i\gamma Bt} + e^{-i\gamma Bt}\right)$$
$$= \tfrac{1}{2}\hbar\sin(2\theta)\cos(\gamma Bt),$$
$$\left\langle S_y\right\rangle = \frac{1}{2}\hbar\begin{pmatrix}e^{-i\gamma Bt/2}\cos\theta & e^{i\gamma Bt/2}\sin\theta\end{pmatrix}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}\begin{pmatrix}e^{i\gamma Bt/2}\cos\theta\\ e^{-i\gamma Bt/2}\sin\theta\end{pmatrix} = \frac{1}{2}\hbar\sin\theta\cos\theta\left(ie^{i\gamma Bt} - ie^{-i\gamma Bt}\right)$$
$$= -\tfrac{1}{2}\hbar\sin(2\theta)\sin(\gamma Bt),$$
$$\left\langle S_z\right\rangle = \frac{1}{2}\hbar\begin{pmatrix}e^{-i\gamma Bt/2}\cos\theta & e^{i\gamma Bt/2}\sin\theta\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}e^{i\gamma Bt/2}\cos\theta\\ e^{-i\gamma Bt/2}\sin\theta\end{pmatrix} = \frac{1}{2}\hbar\left(\cos^2\theta - \sin^2\theta\right)$$
$$= \tfrac{1}{2}\hbar\cos(2\theta).$$

(d) [6] If the spin along the *x*-direction is measured at time *t* what is the probability that it will have the value $+\frac{1}{2}\hbar$?

We need the eigenstates of $S_x = \frac{1}{2}\hbar\sigma_x$, which are $|\pm_x\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ \pm 1\end{pmatrix}$, and the eigenvalues are $\pm\frac{1}{2}\hbar$. The probability of getting $+\frac{1}{2}\hbar$ is

$$P\left(s_x = +\tfrac{1}{2}\hbar\right) = \left|\langle +_x|\Psi(t)\rangle\right|^2 = \left|\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\end{pmatrix}\begin{pmatrix}\cos\theta e^{i\gamma Bt/2}\\ \sin\theta e^{-i\gamma Bt/2}\end{pmatrix}\right|^2 = \frac{1}{2}\left|\cos\theta e^{i\gamma Bt/2} + \sin\theta e^{-i\gamma Bt/2}\right|^2$$

$$= \frac{1}{2}\left(\cos^2\theta + \sin^2\theta + \sin\theta\cos\theta e^{i\gamma Bt} + \sin\theta\cos\theta e^{-i\gamma Bt}\right) = \tfrac{1}{2} + \tfrac{1}{2}\sin(2\theta)\cos(\gamma Bt).$$

(e) [5] The measurement is performed, and the result does come out to be $s_x = +\frac{1}{2}\hbar$. What is the state vector at time t' after the measurement?

At time *t*, the system collapses into the state $|+_x\rangle$, up to an irrelevant phase. Thereafter the components acquire a phase of $e^{\pm i\gamma B(t'-t)/2}$. Therefore, the state at time t' will be

$$|\Psi(t')\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}e^{i\gamma B(t'-t)/2}\\ e^{-i\gamma B(t'-t)/2}\end{pmatrix}.$$

Helpful formulas: $S_i = \frac{1}{2}\hbar\sigma_i, \quad \sigma_x = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}, \quad \sigma_y = \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}, \quad \sigma_z = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}.$

3. A particle of mass *m* in the Harmonic oscillator with frequency ω is in the state $|\psi\rangle = \frac{1}{2}\left(|0\rangle + |1\rangle + \sqrt{2}|2\rangle\right)$

(a) [4] What is the expectation value of the Hamiltonian $\langle H\rangle$?

The states are eigenstates of *H* with eigenvalues $\hbar\omega\left(n+\frac{1}{2}\right)$, so

$$\langle H\rangle = \langle\psi|H|\psi\rangle = \tfrac{1}{4}\left(\langle 0| + \langle 1| + \sqrt{2}\langle 2|\right)H\left(|0\rangle + |1\rangle + \sqrt{2}|2\rangle\right)$$

$$= \tfrac{1}{4}\hbar\omega\left(\langle 0| + \langle 1| + \sqrt{2}\langle 2|\right)\left(\tfrac{1}{2}|0\rangle + \tfrac{3}{2}|1\rangle + \tfrac{5}{2}\sqrt{2}|2\rangle\right) = \tfrac{1}{4}\hbar\omega\left(\tfrac{1}{2} + \tfrac{3}{2} + 5\right) = \tfrac{7}{4}\hbar\omega.$$

(b) [16] What are the expectation values of $\langle X\rangle$, $\langle X^2\rangle$, $\langle P\rangle$, and $\langle P^2\rangle$?

$$\langle X\rangle = \langle\psi|X|\psi\rangle = \frac{1}{4}\sqrt{\frac{\hbar}{2m\omega}}\left(\langle 0|+\langle 1|+\sqrt{2}\langle 2|\right)\left(a+a^\dagger\right)\left(|0\rangle+|1\rangle+\sqrt{2}|2\rangle\right)$$

$$= \frac{1}{4}\sqrt{\frac{\hbar}{2m\omega}}\left(\langle 0|+\langle 1|+\sqrt{2}\langle 2|\right)\left(|1\rangle+|0\rangle+\sqrt{2}|2\rangle+2|1\rangle+\sqrt{6}|3\rangle\right) = \frac{1+3+2}{4}\sqrt{\frac{\hbar}{2m\omega}} = \frac{3}{2}\sqrt{\frac{\hbar}{2m\omega}},$$

$$\langle X^2\rangle = \left\|X|\psi\rangle\right\|^2 = \frac{1}{4}\cdot\frac{\hbar}{2m\omega}\left\|\left(a+a^\dagger\right)\left(|0\rangle+|1\rangle+\sqrt{2}|2\rangle\right)\right\|^2$$

$$= \frac{\hbar}{8m\omega}\left\||1\rangle+|0\rangle+\sqrt{2}|2\rangle+2|1\rangle+\sqrt{6}|3\rangle\right\|^2 = \frac{\hbar}{8m\omega}\left(1^2+3^2+\left(\sqrt{2}\right)^2+\left(\sqrt{6}\right)^2\right) = \frac{9\hbar}{4m\omega},$$

$$\langle P\rangle = \langle\psi|P|\psi\rangle = \frac{i}{4}\sqrt{\frac{\hbar m\omega}{2}}\left(\langle 0|+\langle 1|+\sqrt{2}\langle 2|\right)\left(a^\dagger-a\right)\left(|0\rangle+|1\rangle+\sqrt{2}|2\rangle\right)$$

$$= \frac{i}{4}\sqrt{\frac{\hbar m\omega}{2}}\left(\langle 0|+\langle 1|+\sqrt{2}\langle 2|\right)\left(|1\rangle+\sqrt{2}|2\rangle-|0\rangle+\sqrt{6}|3\rangle-2|1\rangle\right) = \frac{i}{4}\sqrt{\frac{\hbar m\omega}{2}}(-1-1+2) = 0,$$

$$\langle P^2\rangle = \left\|P|\psi\rangle\right\|^2 = \frac{1}{4}\cdot\frac{\hbar m\omega}{2}\left\|i\left(a^\dagger-a\right)\left(|0\rangle+|1\rangle+\sqrt{2}|2\rangle\right)\right\|^2$$

$$= \frac{\hbar m\omega}{8}\left\||1\rangle+\sqrt{2}|2\rangle-|0\rangle+\sqrt{6}|3\rangle-2|1\rangle\right\|^2 = \frac{\hbar m\omega}{8}\left[(-1)^2+(-1)^2+\left(\sqrt{2}\right)^2+\left(\sqrt{6}\right)^2\right] = \frac{5\hbar m\omega}{4}.$$

(c) [5] Find the uncertainties Δx and Δp, and check that it satisfies the uncertainty relation.

The uncertainties are given by

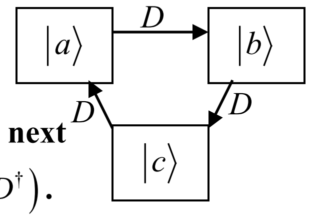
$$\Delta x = \sqrt{\langle X^2\rangle - \langle X\rangle^2} = \sqrt{\frac{\hbar}{m\omega}}\sqrt{\frac{9}{4}-\frac{9}{8}} = \frac{3}{2}\sqrt{\frac{\hbar}{2m\omega}}, \quad \Delta p = \sqrt{\langle P^2\rangle - \langle P\rangle^2} = \sqrt{\hbar m\omega}\sqrt{\frac{5}{4}},$$

$$(\Delta x)(\Delta p) = \frac{3}{4}\sqrt{\frac{5}{2}}\hbar > \tfrac{1}{2}\hbar.$$

Harmonic Oscillator Formulas

$$a|n\rangle = \sqrt{n}|n-1\rangle, \quad a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle, \quad X = \sqrt{\frac{\hbar}{2m\omega}}\left(a+a^\dagger\right), \quad P = i\sqrt{\frac{\hbar m\omega}{2}}\left(a^\dagger-a\right).$$

4. **A quantum mechanical system consists of three orthonormal basis vectors $\{|a\rangle,|b\rangle,|c\rangle\}$, and the operator D is defined by $D|a\rangle=|b\rangle$, $D|b\rangle=|c\rangle$, and $D|c\rangle=|a\rangle$, so that *D* causes each state to "hop" to the next state. The Hamiltonian in this basis is given by $H=-\hbar\omega\left(D^\dagger D+D+D^\dagger\right)$.**



(a) [6] Write the matrix representation of *D*, $D^\dagger$ and *H* in the $\{|a\rangle,|b\rangle,|c\rangle\}$ basis.

The fact that $\langle b|D|a\rangle=1$ tells us that row 2 column 1 of *D* is 1, etc., so we can quickly write down *D* as a matrix. Taking its dagger is trivial, and $D^\dagger D$ is the identity matrix, so we have

$$D=\begin{pmatrix}0&0&1\\1&0&0\\0&1&0\end{pmatrix},\quad D^\dagger=\begin{pmatrix}0&1&0\\0&0&1\\1&0&0\end{pmatrix},\quad H=-\hbar\omega\begin{pmatrix}1&1&1\\1&1&1\\1&1&1\end{pmatrix}.$$

(b) [2] Can the operator *D* correspond to a physical observable? Justify your answer (1 sentence).

D is not Hermitian, and hence cannot correspond to a physical observable.

(c) [6] Show that the states $|\psi_1\rangle=\frac{1}{\sqrt{3}}\left(|a\rangle+|b\rangle+|c\rangle\right)$, $|\psi_2\rangle=\frac{1}{\sqrt{2}}\left(|a\rangle-|b\rangle\right)$, and $|\psi_3\rangle=\frac{1}{\sqrt{6}}\left(|a\rangle+|b\rangle-2|c\rangle\right)$ are eigenstates of the Hamiltonian, and find their eigenvalues.

It is pretty easy to see that these states are orthonormal and that $H=-3\hbar\omega|\psi_1\rangle\langle\psi_1|$. It therefore follows that $H|\psi_1\rangle=-3\hbar\omega|\psi_1\rangle$, while $H|\psi_2\rangle=0$ and $H|\psi_3\rangle=0$.

(d) [11] If the system starts in state $|\Psi(0)\rangle=|c\rangle$ at time 0, what is the state at an arbitrary time $|\Psi(t)\rangle$? If the state is measured at time *t*, what is the probability it will be in the state $|c\rangle$?

It is easy to see that $|\psi_1\rangle-\sqrt{2}|\psi_3\rangle=\sqrt{3}|c\rangle$, so $|\Psi(0)\rangle=\frac{1}{\sqrt{3}}\left(|\psi_1\rangle-\sqrt{2}|\psi_3\rangle\right)$. These eigenstates then just pick up a phase $e^{-iE_it/\hbar}$, so the state at time *t* is

$$|\Psi(t)\rangle=\frac{1}{\sqrt{3}}\left(|\psi_1\rangle e^{3i\omega t}-\sqrt{2}|\psi_3\rangle\right)=\frac{1}{\sqrt{3}}\left[\frac{1}{\sqrt{3}}\begin{pmatrix}1\\1\\1\end{pmatrix}e^{3i\omega t}-\sqrt{\frac{2}{6}}\begin{pmatrix}1\\1\\-2\end{pmatrix}\right]=\frac{1}{3}\begin{pmatrix}e^{3i\omega t}-1\\e^{3i\omega t}-1\\e^{3i\omega t}+2\end{pmatrix}.$$

The probability if it being in the state $|c\rangle$ is then

$$P(c)=\left|\frac{1}{3}\left(e^{3i\omega t}+2\right)\right|^2=\frac{1}{9}\left(e^{3i\omega t}+2\right)\left(e^{-3i\omega t}+2\right)=\frac{1}{9}\left(1+2e^{3i\omega t}+2e^{-3i\omega t}+4\right)=\frac{1}{9}\left[5+4\cos\left(3\omega t\right)\right].$$

5. **Consider a quantum system with just *three* linearly independent states. The Hamiltonian, in matrix form, is**

$$H=V_0\begin{pmatrix}(1-\varepsilon) & 0 & 0\\ 0 & 1 & \varepsilon\\ 0 & \varepsilon & 2\end{pmatrix}$$

Where V_0 is constant and ε is some small parameter ($\varepsilon \ll 1$).

(a) [2] Write down the eigenvectors and eigenvalues of the *unperturbed* Hamiltonian H_0 where $\varepsilon = 0$.

The first step is to simply divide the Hamiltonian into a leading part and a perturbation, which is very easy in this case.

$$H_0=V_0\begin{pmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 2\end{pmatrix} \quad \text{and} \quad W=V_0\begin{pmatrix}-\varepsilon & 0 & 0\\ 0 & 0 & \varepsilon\\ 0 & \varepsilon & 0\end{pmatrix}$$

Since the unperturbed Hamiltonian is diagonal, the three eigenvectors and eigenvalues are trivial. The eigenvectors are

$$|1\rangle=\begin{pmatrix}1\\0\\0\end{pmatrix}, \qquad |2\rangle=\begin{pmatrix}0\\1\\0\end{pmatrix}, \qquad \text{and} \qquad |3\rangle=\begin{pmatrix}0\\0\\1\end{pmatrix}$$

with eigenvalues of V_0, V_0, and $2V_0$ respectively. Hence the third eigenstate is non-degenerate, to this order, and the other two are degenerate.

(b) [5] Use first- and second-order *non*-degenerate perturbation theory to find the approximate eigenvalue for the state that comes from the non-degenerate eigenvector of $\mathbb{H}^0$.

The third eigenstate energy is, to second order in perturbation theory,

$$E_3=E_3^0+\langle 3|W|3\rangle+\sum_{i\neq 3}\frac{\left|\langle i|W|3\rangle\right|^2}{E_3^0-E_i^0}=2V_0+0+\frac{\langle 3|W|2\rangle\langle 2|W|3\rangle}{2V_0-V_0}=2V_0+\frac{\left(\varepsilon V_0\right)^2}{V_0}=V_0\left(2+\varepsilon^2\right).$$

(c) [7] Use *degenerate* perturbation theory to find the first-order correction to the two initially degenerate eigenvalues.

This time things are apparently a little trickier. Because two of the states have the same unperturbed energy, we must use degenerate perturbation theory. To do so, we first work out all matrix elements of the form $W_{ij} = \langle i|W|j\rangle$, where i and j are either of the two degenerate states, so $i, j = 1$ or 2. Looking at the form of the perturbation, the only non-vanishing component of this matrix is $W_{11} = \langle 1|W|1\rangle = -V_0\varepsilon$. So the $\tilde{W}$ W-matrix is

$$\tilde{W} = V_0 \begin{pmatrix} -\varepsilon & 0 \\ 0 & 0 \end{pmatrix},$$

Once again we are lucky, in that the matrix is already diagonalized. This has eigenvalues of $-\varepsilon V_0$ and 0, so we estimate the energies, to first order, as

$$E_1 = V_0(1-\varepsilon) \qquad \text{and} \qquad E_2 = V_0 .$$

These are, however, only accurate to order ε, and we shouldn't be surprised if they turn out to be incorrect at higher order.

(d) [11] Solve for the exact eigenvalues of *H*. Expand each of them as a power series in ε up to second order. Compare with the results of perturbation theory.

The matrix is block diagonal, so we divide it into a 1×1 matrix with eigenvalue $V_0(1-\varepsilon)$, and a remaining 2×2 matrix whose eigenvalues we find from the characteristic equation:

$$0 = \det\begin{pmatrix} 1-x & \varepsilon \\ \varepsilon & 2-x \end{pmatrix} = (1-x)(2-x) - \varepsilon^2 = x^2 - 3x + 2 - \varepsilon^2$$

Using the quadratic formula, the roots of this are $x = \tfrac{1}{2}\left(3 \pm \sqrt{9-8+4\varepsilon^2}\right) = \tfrac{1}{2}\left(3 \pm \sqrt{1+4\varepsilon^2}\right)$.

Multiplying these back by the common factor of V_0, and using the binomial expansion to approximate $\sqrt{1+4\varepsilon^2} \approx 1 + 2\varepsilon^2 - 2\varepsilon^4$, we then find the eigenvalues

$$E_1 = V_0(1-\varepsilon),$$
$$E_2 = \tfrac{1}{2}V_0\left(3 - \sqrt{1+4\varepsilon^2}\right) \approx V_0\left(1 - \varepsilon^2 + \varepsilon^4\right),$$
$$E_3 = \tfrac{1}{2}V_0\left(3 + \sqrt{1+4\varepsilon^2}\right) \approx V_0\left(2 + \varepsilon^2 - \varepsilon^4\right).$$

Comparing with the results we got before, we see that we got E_1 exactly right, for E_2 we missed the second order term (since we didn't do second order perturbation theory), and for E_3 we got the second order term but missed the next (fourth-order) term.