## Physics 742 – Graduate Quantum Mechanics 2 Solutions to Second Exam, Spring 2023

The points for each question are marked. Each question is worth 20 points. Some possibly useful formulas appear at the end of the test or on the handout.

A particle of mass *m* is in the ground state of a 3D harmonic oscillator with time-dependent frequency, so V(r,t) = ½mω²(t)r². At t = -∞, ω(t) = ω₀, while at t = +∞, ω(t) = 2ω₀. What is the probability it ends in the ground state if the process is (a) adiabatic, or (b) sudden?

Obviously, the ground state has the minimum energy. The potential can be written in the form  $V(\mathbf{r},t) = \frac{1}{2}m\omega^2(t)(x^2 + y^2 + z^2)$ , so the potential can be split into three separate Hamiltonians, and the resulting wave function will be of the form of products of wave functions in the three dimensions. At both the beginning and the end, we therefore have

$$\psi(\mathbf{r}) = \psi_0(x)\psi_0(y)\psi_0(z) = \left(\frac{m\omega}{\pi\hbar}\right)^{3/4} \exp\left[-\frac{m\omega}{2\hbar}\left(x^2 + y^2 + z^2\right)\right] = \left(\frac{m\omega}{\pi\hbar}\right)^{3/4} e^{-m\omega r^2/2\hbar}$$

The only difference between the initial ground state and the final state is that the value of  $\omega$  changes from  $\omega_0$  to  $2\omega_0$ , so we have

$$\psi_{g}(\mathbf{r}) = \left(\frac{m\omega_{0}}{\pi\hbar}\right)^{3/4} e^{-m\omega_{0}r^{2}/2\hbar} \text{ and } \psi_{g}'(\mathbf{r}) = \left(\frac{m2\omega_{0}}{\pi\hbar}\right)^{3/4} e^{-m\omega_{0}r^{2}/2}.$$

In the adiabatic approximation, the ground state evolves to the ground state, so we would have  $P(|\psi_g\rangle \rightarrow |\psi'_g\rangle) = 1$ . In the sudden approximation, the probability is given by the square of the magnitude of the inner product of the two states, so

$$P(|\psi_{g}\rangle \rightarrow |\psi_{g}'\rangle) = |\langle\psi_{g}'|\psi_{g}\rangle|^{2} = |\int d^{3}\mathbf{r}\,\psi_{g}'^{*}(\mathbf{r})\psi_{g}(\mathbf{r})|^{2}$$

$$= \left|\left(\frac{m\omega_{0}}{\pi\hbar}\right)^{3/4}\left(\frac{m2\omega_{0}}{\pi\hbar}\right)^{3/4}\int d\Omega \int_{0}^{\infty} e^{-m\omega_{0}r^{2}/2\hbar}e^{-m\omega_{0}r^{2}/\hbar}r^{2}dr\right|^{2}$$

$$= \left|\left(\frac{m\omega_{0}}{\pi\hbar}\right)^{3/2}2^{3/4}4\pi \int_{0}^{\infty} e^{-3m\omega_{0}r^{2}/2\hbar}r^{2}dr\right|^{2} = \left[\left(\frac{m\omega_{0}}{\pi\hbar}\right)^{3/2}2^{3/4}4\pi \left(\frac{2\hbar}{3m\omega_{0}}\right)^{3/2}\frac{1}{2}\Gamma\left(\frac{3}{2}\right)\right]^{2}$$

$$= \left[2^{3/4}4\pi \left(\frac{2}{3\pi}\right)^{3/2}\frac{1}{2}\cdot\frac{\sqrt{\pi}}{2}\right]^{2} = \left(\frac{2^{9/4}}{3^{3/2}}\right)^{2} = \frac{16\sqrt{2}}{27} \approx 83.8\%.$$

2. A particle is in the ground state  $|0,0,0\rangle$  of a 3D harmonic oscillator with frequency  $\omega_0$ . A perturbation of the form  $W = \alpha XYZ$  is turned on at time t = 0. Find the probability to leading (second) order in  $\alpha$  that it is in some other state at time T.

We need the effect of the perturbation on the state, which is given by

$$W|0,0,0\rangle = \alpha XYZ|0,0,0\rangle = \alpha \left(\frac{\hbar}{2m\omega_0}\right)^{3/2} \left(a_x + a_x^{\dagger}\right) \left(a_y + a_y^{\dagger}\right) \left(a_z + a_z^{\dagger}\right) |0,0,0\rangle$$
$$= \alpha \left(\frac{\hbar}{2m\omega_0}\right)^{3/2} \left(a_x + a_x^{\dagger}\right) \left(a_y + a_y^{\dagger}\right) |0,0,1\rangle = \alpha \left(\frac{\hbar}{2m\omega_0}\right)^{3/2} \left(a_x + a_x^{\dagger}\right) |0,1,1\rangle$$
$$= \left(\frac{\hbar}{2m\omega_0}\right)^{3/2} |1,1,1\rangle$$

To leading order, the only state that can be excited is therefore  $|1,1,1\rangle$ . We need the matrix element  $W_{FI}(t) = W_{111,000}(t)$ , which is simply  $(\hbar/2m\omega_0)^{3/2}$ . The scattering amplitude is given in this case given by just  $S_{FI} = (i\hbar)^{-1} \int_0^T dt W_{FI}(t) e^{i\omega_{FI}t}$ . We will need the frequency difference, which is

$$\omega_{FI} = \frac{E_{111} - E_{000}}{\hbar} = \frac{\hbar \omega_0 \left(1 + 1 + 1 + \frac{3}{2}\right) - \frac{3}{2} \hbar \omega_0}{\hbar} = 3\omega_0.$$

We therefore have a scattering matrix element of

$$S_{FI} = \frac{1}{i\hbar} \int_{0}^{T} dt W_{FI}(t) e^{i\omega_{FI}t} = \frac{\alpha}{i\hbar} \left(\frac{\hbar}{2m\omega_{0}}\right)^{3/2} \int_{0}^{T} e^{3i\omega_{0}t} dt = \frac{\alpha}{i\hbar} \left(\frac{\hbar}{2m\omega_{0}}\right)^{3/2} \frac{1}{3i\omega_{0}} e^{3i\omega_{0}t} \Big|_{0}^{T}$$
$$= \frac{\alpha\sqrt{\hbar}}{3(2m)^{3/2} \omega_{0}^{5/2}} \left(1 - e^{3i\omega_{0}T}\right).$$

The probability of a transition is just the square of the magnitude of this expression, so

$$P(|000\rangle \rightarrow |111\rangle) = |S_{FI}|^{2} = S_{FI}^{*}S_{FI} = \frac{\alpha^{2}\hbar}{9 \cdot 8m^{3}\omega_{0}^{5}}(1 - e^{-3i\omega_{0}T})(1 - e^{3i\omega_{0}T})$$
$$= \frac{\alpha^{2}\hbar}{72m^{3}\omega_{0}^{5}}(1 - e^{-3i\omega_{0}T} - e^{3i\omega_{0}T} + 1) = \frac{\alpha^{2}\hbar}{72m^{3}\omega_{0}^{5}}[2 - 2\cos(3\omega_{0}T)]$$
$$= \frac{\alpha^{2}\hbar}{36m^{3}\omega_{0}^{5}}[1 - \cos(3\omega_{0}T)].$$

**3.** Suppose that we have a solution  $\Psi(\mathbf{r},t)$  of the free Dirac equation, so

 $i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{r},t) = (-i\hbar c \mathbf{a} \cdot \nabla + mc^2 \beta) \Psi(\mathbf{r},t)$ . Show that  $\Psi(-\mathbf{r},t)$  is generally *not* a solution, but that  $\beta \Psi(-\mathbf{r},t)$  is, where  $\beta$  is the matrix appearing in the Dirac equation.

We start by simply substituting  $\Psi(-\mathbf{r},t)$  in, and then seeing if we can turn it back into the starting equation. We start with

$$i\hbar \frac{\partial}{\partial t} \Psi(-\mathbf{r},t) = (-i\hbar c \mathbf{a} \cdot \nabla + mc^2 \beta) \Psi(-\mathbf{r},t).$$

We now let  $\mathbf{r} \rightarrow -\mathbf{r}$  everywhere in this equation, but keeping track of the fact that the gradient will change sign in the process. We therefore claim this equation is equivalent to

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{r},t) = (i\hbar c \mathbf{a} \cdot \nabla + mc^2 \beta) \Psi(\mathbf{r},t).$$

This obviously failed.

We try again, but this time substituting  $\beta \Psi(-\mathbf{r},t)$ , so we have

$$i\hbar \frac{\partial}{\partial t} \beta \Psi(-\mathbf{r},t) = (-i\hbar c \mathbf{a} \cdot \nabla + mc^2 \beta) \beta \Psi(-\mathbf{r},t).$$

We again substitute  $\mathbf{r} \rightarrow -\mathbf{r}$  everywhere, so we have

$$i\hbar \frac{\partial}{\partial t} \beta \Psi(\mathbf{r},t) = (i\hbar c \mathbf{a} \cdot \nabla + mc^2 \beta) \beta \Psi(\mathbf{r},t).$$

We would like to bring the  $\beta$ 's to the left. This can be done on the left, and since  $\beta$  obviously commutes with itself, it can also be done on the last term on the right. However, because  $\alpha_i\beta = -\beta\alpha_i$ , we must change the sign on the first term on the right, so we have

$$\beta i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{r},t) = \beta \left(-i\hbar c \mathbf{a} \cdot \nabla + mc^2 \beta\right) \Psi(\mathbf{r},t).$$

We now simply wish to "cancel" the factor of  $\beta$  on both sides. This can be done most clearly by multiplying by  $\beta$  on the left of both sides and using  $\beta^2 = 1$  to yield

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{r},t) = (-i\hbar c \mathbf{a} \cdot \nabla + mc^2 \beta) \Psi(\mathbf{r},t),$$

This is the original Dirac equation, so our argument has been proven.

4. An electromagnetic system is in a superposition of zero or one photons state,  $|\psi\rangle = N(\sqrt{2}|0\rangle + |1,q,1\rangle + i|1,q,2\rangle)$ , where  $\mathbf{q} = q\hat{\mathbf{z}}$ ,  $\varepsilon_{q1} = \hat{\mathbf{x}}$  and  $\varepsilon_{q2} = \hat{\mathbf{y}}$ . Find the normalization N and the electric field expectation value  $\langle \psi | \mathbf{E}(\mathbf{r}) | \psi \rangle$ . Your final answer should be manifestly real.

The normalization can be found by demanding that

$$1 = \langle \psi | \psi \rangle = N^* N \left( \sqrt{2} \langle 0 | + \langle 1, \mathbf{q}, 1 | -i \langle 1, \mathbf{q}, 2 | \right) \left( \sqrt{2} | 0 \rangle + |1, \mathbf{q}, 1 \rangle + i | 1, \mathbf{q}, 2 \rangle \right) = N^* N (2 + 1 + 1).$$
  
$$4 |N|^2 = 1.$$

Up to an irrelevant phase, this means that  $N = \frac{1}{2}$ . We then compute the electric field using

$$\langle \psi | \mathbf{E}(\mathbf{r}) | \psi \rangle = \frac{i}{4} \sum_{\mathbf{k},\sigma} \left( \sqrt{2} \langle 0 | + \langle 1, \mathbf{q}, 1 | -i \langle 1, \mathbf{q}, 2 | \right) \sqrt{\frac{\hbar \omega_k}{2\varepsilon_0 V}} \left( a_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}\sigma} e^{i\mathbf{k}\cdot\mathbf{r}} - a_{\mathbf{k}\sigma}^{\dagger} \varepsilon_{\mathbf{k}\sigma}^{*} e^{-i\mathbf{k}\cdot\mathbf{r}} \right)$$
$$\left( \sqrt{2} | 0 \rangle + | 1, \mathbf{q}, 1 \rangle + i | 1, \mathbf{q}, 2 \rangle \right).$$

The electric field operator either adds or subtracts one photon, and there is only zero or one photon on the left of the right. The only non-zero terms will be either when we start with no photons and create one, or we start with one photon and end with zero, so we have

$$\langle \psi | \mathbf{E}(\mathbf{r}) | \psi \rangle = \frac{i}{4} \sum_{\mathbf{k},\sigma} \sqrt{\frac{\hbar \omega_k}{2\varepsilon_0 V}} \begin{bmatrix} \sqrt{2} \langle 0 | a_{\mathbf{k}\sigma} \mathbf{\varepsilon}_{\mathbf{k}\sigma} e^{i\mathbf{k}\cdot\mathbf{r}} (|1,\mathbf{q},1\rangle + i|1,\mathbf{q},2\rangle) \\ -\sqrt{2} (\langle 1,\mathbf{q},1| - i\langle 1,\mathbf{q},2| \rangle) a_{\mathbf{k}\sigma}^{\dagger} \mathbf{\varepsilon}_{\mathbf{k}\sigma}^{*} e^{-i\mathbf{k}\cdot\mathbf{r}} | 0 \rangle \end{bmatrix}.$$

The only value of **k** that contributes is  $\mathbf{k} = \mathbf{q}$ , so we collapse this sum. We also write out the polarization sums explicitly as two terms. We then use  $\langle 0 | a_{\mathbf{q}\sigma} | 1, \mathbf{q}, \tau \rangle = \langle 0 | a_{\mathbf{q}\sigma}^{\dagger} | 1, \mathbf{q}, \tau \rangle = \delta_{\sigma\tau}$  to simplify, which turns this into

$$\begin{aligned} \left\langle \psi \left| \mathbf{E}(\mathbf{r}) \right| \psi \right\rangle &= \frac{i}{4} \sqrt{\frac{\hbar \omega_q}{\varepsilon_0 V}} \sum_{\sigma} \begin{bmatrix} e^{i\mathbf{q}\cdot\mathbf{r}} \left\langle 0 \right| \left( a_{q1} \hat{\mathbf{x}} + a_{q2} \hat{\mathbf{y}} \right) \left( |1, \mathbf{q}, 1\rangle + i |1, \mathbf{q}, 2\rangle \right) \\ &- e^{-i\mathbf{q}\cdot\mathbf{r}} \left( \left\langle 1, \mathbf{q}, 1 \right| - i \left\langle 1, \mathbf{q}, 2 \right| \right) \left( a_{q1}^{\dagger} \hat{\mathbf{x}} + a_{q2}^{\dagger} \hat{\mathbf{y}} \right) |0\rangle \end{bmatrix} \\ &= \frac{i}{4} \sqrt{\frac{\hbar c q}{\varepsilon_0 V}} \left[ e^{iqz} \left( \hat{\mathbf{x}} + i \hat{\mathbf{y}} \right) - e^{-iqz} \left( \hat{\mathbf{x}} - i \hat{\mathbf{y}} \right) \right] \\ &= \frac{1}{4} \sqrt{\frac{\hbar c q}{\varepsilon_0 V}} \left[ \hat{\mathbf{x}} i \left( e^{iqz} - e^{-iqz} \right) - \hat{\mathbf{y}} \left( e^{iqz} + e^{-iqz} \right) \right] \\ &= \frac{1}{2} \sqrt{\frac{\hbar c q}{\varepsilon_0 V}} \left[ -\hat{\mathbf{x}} \sin(qz) - \hat{\mathbf{y}} \cos(qz) \right]. \end{aligned}$$

The final answer is manifestly real.

5. An electron of mass *m* is in a 3D cubical infinite square well of size *a* in the state  $|n_x, n_y, n_z\rangle = |4, 1, 1\rangle$ . Find the dipole matrix element  $\mathbf{r}_{FI}$  between this and any of the lower energy states  $|n, 1, 1\rangle$ , and the rate  $\Gamma$  to decay to each of these states.

The eigenstates of the 3D infinite square well are of the form  $|n_x, n_y, n_z\rangle$ , and they have wave functions and energies of

$$\psi_{n_x,n_y,n_z} = \sqrt{\frac{8}{a^3}} \sin\left(\frac{\pi n_x x}{a}\right) \sin\left(\frac{\pi n_y y}{a}\right) \sin\left(\frac{\pi n_z z}{a}\right), \quad E_{n_x,n_y,n_z} = \frac{\pi^2 \hbar^2 \left(n_x^2 + n_y^2 + n_z^2\right)}{2ma}$$

We are supposed to only go down in energy, so we assume n < 4, so there are only three cases, n = 1, 2, and 3.

In the dipole approximation we need to calculate the  $\mathbf{r}_{FI} = \langle F | \mathbf{R} | I \rangle$ . If we calculate some component other than *x*, then the *x*-integral will yield  $\int_0^a \sin(n\pi x/a)\sin(4\pi x/a)dx = 0$ . So the only non-zero components will be the *x*-components, for which we have

$$\mathbf{r}_{FI} = \hat{\mathbf{x}} \langle n, 1, 1 | Y | 4, 1, 1 \rangle = \hat{\mathbf{x}} \frac{8}{a^3} \int_0^a x \sin\left(\frac{n\pi x}{a}\right) \sin\left(\frac{4\pi x}{a}\right) dx \int_0^a \sin^2\left(\frac{\pi y}{a}\right) dy \int_0^a \sin^2\left(\frac{\pi z}{a}\right) dz$$
$$= \hat{\mathbf{x}} \frac{8}{a^3} \left\{ \frac{-2a^2 4n \left[1 - (-1)^{n+4}\right]}{\pi^2 \left(n^2 - 4^2\right)^2} \right\} \frac{a}{2} \cdot \frac{a}{2} = -a \hat{\mathbf{x}} \frac{16n \left[1 - (-1)^n\right]}{\pi^2 \left(n^2 - 16\right)^2}.$$

The only non-zero values are when n is odd, so we have

$$\mathbf{r}_{111,411} = -a\hat{\mathbf{x}}\frac{32}{225\pi^2}$$
 and  $\mathbf{r}_{311,411} = -a\hat{\mathbf{x}}\frac{96}{49\pi^2}$ 

We will also need the frequencies in each case, which are

$$\omega_{411,111} = \frac{1}{\hbar} \left( E_{411} - E_{111} \right) = \frac{1}{\hbar} \frac{\pi^2 \hbar^2}{2ma^2} \left( 4^2 - 1^2 \right) = \frac{15\pi^2 \hbar}{2ma^2},$$
  
$$\omega_{411,311} = \frac{1}{\hbar} \left( E_{411} - E_{311} \right) = \frac{1}{\hbar} \frac{\pi^2 \hbar^2}{2ma^2} \left( 4^2 - 3^2 \right) = \frac{7\pi^2 \hbar}{2ma^2}.$$

We now substitute into the formula for spontaneous decay via dipole moment to find

$$\Gamma(|411\rangle \rightarrow |111\rangle) = \frac{4\alpha}{3c^2} \omega_{411,111}^3 |\mathbf{r}_{111,411}|^2 = \frac{4\alpha}{3c^2} \left(\frac{15\pi^2\hbar}{2ma^2}\right)^3 \left(-\frac{32a}{225\pi^2}\right)^2 = \frac{512\pi^2\alpha\hbar^3}{45m^3c^2a^4},$$
  
$$\Gamma(|411\rangle \rightarrow |311\rangle) = \frac{4\alpha}{3c^2} \omega_{411,311}^3 |\mathbf{r}_{311,411}|^2 = \frac{4\alpha}{3c^2} \left(\frac{7\pi^2\hbar}{2ma^2}\right)^3 \left(-\frac{96a}{49\pi^2}\right)^2 = \frac{1536\pi^2\alpha\hbar^3}{7m^3c^2a^4}.$$

One could continue and find the branching ratio, which in this case works out to  $\frac{7}{142}$  for the first one and  $\frac{135}{142}$  for the second, but I'm glad I didn't ask for that.

1D harmonic oscillator: $V(x) = \frac{1}{2}m\omega^{2}x^{2}$	Time-dependent Perturbation Theory $S_{FI} = \delta_{FI} + \frac{1}{i\hbar} \int_{0}^{T} dt W_{FI}(t) e^{i\omega_{FI}t} + \cdots$		Trigonometry $\cos(\theta) = \frac{1}{2} \left( e^{i\theta} + e^{-i\theta} \right)$
$X = \sqrt{\frac{\hbar}{2m\omega}} (a + a^{\dagger})$ $a   n \rangle = \sqrt{n}   n - 1 \rangle$ $a^{\dagger}   n \rangle = \sqrt{n+1}   n+1 \rangle$	$\alpha^2 - \beta^2 - 1$	Spontaneous Decay $\Gamma = \frac{4\alpha}{3c^2} \omega_{IF}^3 \left  \mathbf{r}_{FI} \right ^2$	a (a)
$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-m\omega x^2/2\hbar}$	Electric field operator $\mathbf{E}(\mathbf{r}) = \sum_{\mathbf{k},\sigma} \sqrt{\frac{\hbar \omega_k}{2\varepsilon_0 V}} i \left( a_{\mathbf{k}\sigma} \mathbf{\varepsilon}_{\mathbf{k}\sigma} e^{i\mathbf{k}\cdot\mathbf{r}} - a_{\mathbf{k}\sigma}^{\dagger} \mathbf{\varepsilon}_{\mathbf{k}\sigma}^* e^{-i\mathbf{k}\cdot\mathbf{r}} \right)$		$E_n = \frac{\pi^2 n^2 \hbar^2}{2ma^2}$

## **Possibly Helpful Formulas:**

**Possibly Helpful Integrals:** The formulas below assume *n* and *p* are non-negative integers  $\Gamma(n+1)$ 

$$\int_{0}^{\infty} x^{n} e^{-Ax^{2}} dx = \frac{\Gamma(n+\frac{1}{2})}{2A^{n+\frac{1}{2}}}, \quad \Gamma(\frac{1}{2}) = \sqrt{\pi}, \quad \Gamma(1) = 1, \quad \Gamma(\frac{3}{2}) = \frac{1}{2}\sqrt{\pi}, \quad \Gamma(2) = 1, \quad \Gamma(\frac{5}{2}) = \frac{3}{4}\sqrt{\pi}.$$

$$\int_{0}^{a} \sin\left(\frac{\pi nx}{a}\right) \sin\left(\frac{\pi px}{a}\right) dx = \frac{1}{2}a\delta_{np}, \quad \int_{0}^{a} x\sin\left(\frac{\pi nx}{a}\right) \sin\left(\frac{\pi px}{a}\right) dx = \frac{-2a^{2}pn\left[1-(-1)^{n+p}\right]}{\pi^{2}\left(n^{2}-p^{2}\right)^{2}}.$$