

Assignment 2: Identical particles, transitions, and density matrices

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Exercise 1 *Multiparticle harmonic oscillator* (20 points)

Consider two non-interacting particles of mass m in the harmonic oscillator potential well. For the case with one particle in the single-particle state $|n\rangle$ and the other in state $|k\rangle$ (where $n \neq k$), we are going to calculate the expectation value of the squared interparticle spacing: $\langle (x_1 - x_2)^2 \rangle$. Do this for the cases where the particles are:

- distinguishable
- spin-0
- spin-1/2 in a spin triplet state

In all cases, calculate the expected interparticle spacing and explain whether the results are consistent with your expectations, and why.

Hint Use Dirac notation: with the correct application, integration is not required for the above calculations. Go forth and harness the power of state vectors to improve your quality of life!

Exercise 2 *Helium ground state energy* (11 points)

- (9 marks) Compute the direct integral for the ground state of helium and show the first-order correction to the energy is $E_{1s,1s}^{(1)} = \frac{5}{2}\text{Ry} = 34\text{eV}$.

Hint: For no reason, here is the *spherical harmonic addition theorem*:

$$\frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \frac{4\pi}{2\ell+1} \frac{r_{<}^{\ell}}{r_{>^{\ell+1}}} Y_{\ell}^{m*}(\theta_1, \phi_1) Y_{\ell}^m(\theta_2, \phi_2)$$

where $r_{>}/r_{<}$ denoting the larger/smaller of the two distances r_1 and r_2 , will make this problem easier.

- (2 marks) Imagine that we are back in week one, where the variational method was introduced. If we had guessed that the wave function of helium was roughly

$$\psi_{He} = \varphi_{nlm}(\mathbf{r}_1)\varphi_{nlm}(\mathbf{r}_2)$$

where $\varphi_{nlm}(\mathbf{r})$ are the usual hydrogenic wave functions, explain why we would have calculated the identical result to that above, assuming that the interaction potential between electrons was the same. You can incorporate into your answer why I am nice for not having asked you to calculate the ground state energy for a trial wave function *not* of that form, for example, if $\varphi(\mathbf{r}) = \exp -\alpha(r_1 - r_2)^2$.

Exercise 3 *Density of states* (12 points)

In class, it was stated that the density of states $g(E)$ can be calculated as the Fourier transform of the emitted field, and for an exponentially decaying excited state, the density of states is

$$g(E) = \frac{\hbar A_{21}/2\pi}{(E - \hbar\omega_{12})^2 + \left(\frac{\hbar A_{21}}{2}\right)^2}$$

We are going to show exactly this.

1. (1 mark) Explain why that given a population which decays exponentially with time dependence $e^{-t/\tau}$, the field decays with the a time dependence $e^{-t/2\tau}$.
2. (4 marks) Calculate the Fourier transform of the emitted field,

$$E(t) = \begin{cases} 0 & t < 0 \\ E_0 e^{-t/2\tau} e^{-i\omega_{21}t} & t \geq 0 \end{cases}$$

and hence find the frequency spectrum of the radiated power in spontaneous emission.

Hint: The power spectral density is computed as the square of the absolute value of the Fourier transform.

3. (4 marks) Convert this frequency spectrum to an energy spectrum, and normalise it (to 1) and *voilà*, you should arrive at the density of states above.

Hint: You will need to make the (very valid) approximation that the linewidth A_{21} is much less than the resonance frequency ω_{21}

Exercise 4 *Absorption of light* (11 points)

Light of frequency ω propagates in the z direction and is incident on an ensemble of two-level atoms. In the steady state, we can model the absorption process by assuming that the intensity falls off as $I(z) = I_0 e^{-\alpha z}$.

1. (2 marks) Show that $\alpha = k \text{Im}[\chi]$ where k is the wavenumber
2. (4 marks) Show that in the case of homogeneous broadening, the absorption per unit length is given by

$$\frac{dI}{dz} = -\frac{k I n d_{12}^2}{\epsilon_0 \hbar} \frac{\Gamma}{2} \frac{1}{\Delta^2 + \frac{\Gamma^2}{4} + \frac{\Omega^2}{2}}$$

3. (3 marks) Assuming resonant conditions, by introducing the on-resonance saturation parameter, $s_0 = \frac{2\Omega^2}{\Gamma^2}$, derive the *Beer-Lambert law*:

$$\frac{1}{I} \frac{dI}{dz} = -\frac{n\hbar\omega}{I_{sat}} \frac{\Gamma}{2}$$

where $\frac{I}{I_{sat}} = s_0$.

4. (2 marks) In the high-intensity limit ($s \rightarrow \infty$), this reduces to

$$\frac{dI}{dz} = -n\hbar\omega \frac{\Gamma}{2}.$$

Comment on the significance of this, in particular, what happens to the transmission as a function of light as a function of incident intensity?

Exercise 5 *The density matrix and OBEs* (25 points)

Here we are going to compute some density matrices, and then we are going to solve the optical Bloch equations.

1. (2 marks) What is the density matrix for the state $\psi = 0.577|+\rangle + 0.577(1+i)|-\rangle$ in the $|\pm\rangle$ basis?
2. (1 mark) What is the expectation value for S_y ?
3. (1 mark) What is a mixed state which would give the same probabilities of measuring the system in states $|+\rangle$ and $|-\rangle$?
4. (2 marks) Explain why we care about the difference between pure and mixed states, and what differences one might observe in experiments when using either a pure or mixed state

`\begin{Computational content}`

The computation of density matrices can be tedious, especially once we have larger systems. Consider the state

$$|\psi\rangle = \frac{1}{\sqrt{10}} (3|++\rangle + 1|+-\rangle + 4|-+\rangle + 2|--\rangle)$$

in the basis $|J_1 J_2 m_{J_1} m_{J_2}\rangle$, where $J_1, J_2 = 1/2$ and have been dropped from the state labels.

Using **Python** (or equivalent)

1. (3 marks) Compute the density matrix ρ for the above state $|\psi\rangle$
2. (3 marks) Compute the expectation value $\langle \mathbf{F}^2 \rangle$ for this state

We now turn to the optical Bloch equations. We have seen that in the rotating wave approximation, we can solve them analytically, but such approximations are not always valid, but more generally, in large systems the analytical solutions become nightmarish (e.g. see appendix D of [my Ph.D thesis](#)). Consequently, we seek to solve them numerically.

Using **Python**

1. (8 marks) Compute and plot the evolution of the matrix elements $\rho_{11}, \rho_{12}, \rho_{21}$, and ρ_{22} as a function of time for realistic experimental parameters.

Hint: This means that you will need to figure out what realistic parameters are.

2. (5 marks) Use the computational package **QuTiP** to produce plots of the same matrix elements.

Hint: This is an exercise to demonstrate that using established libraries can make complex tasks simple, and thus should not require any complex computation *per se*.

As computational experience, competence, and confidence will vary across the class, I have provided a [jupyter notebook](#) to provide a few hot tips.