PSET 1

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1 Problem 1: Adjoint Operators and Turnover Rule (10 points)

1.0.1 Question

Two operators $\hat{O}$ and $\hat{O}^\dagger$ are defined to be adjoint if their expectation values are complex conjugates of one another. That is:

$$\langle\phi|\hat{O}^\dagger|\phi\rangle = \langle\phi|\hat{O}|\phi\rangle^*$$

and

$$(\hat{O}^\dagger)^\dagger = \hat{O}$$

Consider two functions ϕ_1 and ϕ_2 in the domain of adjoint operators $\hat{O}$ and $\hat{O}^\dagger$. Two new functions in this domain, Φ_A and Φ_B, are given by

$$\Phi_A = \phi_1 + \phi_2$$
$$\Phi_B = \phi_1 + i\phi_2$$

where $i = \sqrt{-1}$. Use the definition of adjoint operators to prove the turnover rule:

$$\langle\phi_1|\,\hat{O}^\dagger\,|\phi_2\rangle = \left\langle \hat{O}\phi_1 \middle| \phi_2 \right\rangle$$

Some important properties: if z_1 and z_2 are two different complex numbers, then $z_1^* z_2 = (z_2 z_1^*)^*$; $z^\dagger = z^*$; $\langle u|^\dagger = |u\rangle$; $\langle u_1|u_2\rangle^\dagger = \langle u_1|u_2\rangle^* = \langle u_2|u_1\rangle$.

1.0.2 Answer

We consider

$$\langle\Phi_A|\,\hat{O}^\dagger\,|\Phi_A\rangle = \langle\Phi_A|\,\hat{O}\,|\Phi_A\rangle^* \tag{1}$$

and

$$\langle\Phi_B|\,\hat{O}^\dagger\,|\Phi_B\rangle = \langle\Phi_B|\,\hat{O}\,|\Phi_B\rangle^* \tag{2}$$

We insert that expressions for Φ_A and Φ_B. For the first one, we have:

$$\langle\phi_1+\phi_2|\,\hat{O}^\dagger\,|\phi_1+\phi_2\rangle = \langle\phi_1+\phi_2|\,\hat{O}\,|\phi_1+\phi_2\rangle^* \tag{3}$$

Expanding both sides:

$$\langle\phi_1|\,\hat{O}^\dagger\,|\phi_1\rangle+\langle\phi_2|\,\hat{O}^\dagger\,|\phi_2\rangle+\langle\phi_1|\,\hat{O}^\dagger\,|\phi_2\rangle+\langle\phi_2|\,\hat{O}^\dagger\,|\phi_1\rangle = \Big(\langle\phi_1|\,\hat{O}\,|\phi_1\rangle + \langle\phi_2|\,\hat{O}\,|\phi_2\rangle + \langle\phi_1|\,\hat{O}\,|\phi_2\rangle + \langle\phi_2|\,\hat{O}\,|\phi_1\rangle\Big)^* \tag{4}$$

Distributing out the complex conjugation:

$$\langle\phi_1|\,\hat{O}^\dagger\,|\phi_1\rangle+\langle\phi_2|\,\hat{O}^\dagger\,|\phi_2\rangle+\langle\phi_2|\,\hat{O}^\dagger\,|\phi_1\rangle+\langle\phi_1|\,\hat{O}^\dagger\,|\phi_2\rangle = \langle\phi_1|\,\hat{O}\,|\phi_1\rangle^*+\langle\phi_2|\,\hat{O}\,|\phi_2\rangle^*+\langle\phi_2|\,\hat{O}\,|\phi_1\rangle^*+\langle\phi_1|\,\hat{O}\,|\phi_2\rangle^* \tag{5}$$

We can cancel out the first two terms from either side:

$$\langle\phi_2|\,\hat{O}^\dagger\,|\phi_1\rangle + \langle\phi_1|\,\hat{O}^\dagger\,|\phi_2\rangle = \langle\phi_2|\,\hat{O}\,|\phi_1\rangle^* + \langle\phi_1|\,\hat{O}\,|\phi_2\rangle^* \tag{6}$$

For the second one, we have:

$$\langle\phi_1 + i\phi_2|\,\hat{O}^\dagger\,|\phi_1 + i\phi_2\rangle = \langle\phi_1 + i\phi_2|\,\hat{O}\,|\phi_1 + i\phi_2\rangle^* \tag{7}$$

Expanding both sides:

$$\begin{gathered}\langle\phi_1|\,\hat{O}^\dagger\,|\phi_1\rangle + \langle\phi_2|\,\hat{O}^\dagger\,|\phi_2\rangle + i\,\langle\phi_1|\,\hat{O}^\dagger\,|\phi_2\rangle - i\,\langle\phi_2|\,\hat{O}^\dagger\,|\phi_1\rangle = \\ \Big(\langle\phi_1|\,\hat{O}\,|\phi_1\rangle + \langle\phi_2|\,\hat{O}\,|\phi_2\rangle + i\,\langle\phi_1|\,\hat{O}\,|\phi_2\rangle - i\,\langle\phi_2|\,\hat{O}\,|\phi_1\rangle\Big)^*\end{gathered}$$

Distributing out the complex conjugation:

$$\langle\phi_1|\,\hat{O}^\dagger\,|\phi_1\rangle+\langle\phi_2|\,\hat{O}^\dagger\,|\phi_2\rangle+i\,\langle\phi_1|\,\hat{O}^\dagger\,|\phi_2\rangle-i\,\langle\phi_2|\,\hat{O}^\dagger\,|\phi_1\rangle = \langle\phi_1|\,\hat{O}\,|\phi_1\rangle^*+\langle\phi_2|\,\hat{O}\,|\phi_2\rangle^*-i\,\langle\phi_1|\,\hat{O}\,|\phi_2\rangle^*+i\,\langle\phi_2|\,\hat{O}\,|\phi_1\rangle^* \tag{8}$$

We can cancel out the first two terms from both sides:

$$i\,\langle\phi_1|\,\hat{O}^\dagger\,|\phi_2\rangle - i\,\langle\phi_2|\,\hat{O}^\dagger\,|\phi_1\rangle = -i\,\langle\phi_1|\,\hat{O}\,|\phi_2\rangle^* + i\,\langle\phi_2|\,\hat{O}\,|\phi_1\rangle^* \tag{9}$$

Multiplane through equation 6 by i and adding it to 9, then dividing the result by $2i$, we get:

$$\langle\phi_1|\,\hat{O}^\dagger\,|\phi_2\rangle = \langle\phi_2|\,\hat{O}\,|\phi_1\rangle^* \tag{10}$$

So, we have shown the turnover rule that:

$$\langle\phi_1|\,\hat{O}^\dagger\,|\phi_2\rangle = \Big\langle\hat{O}\phi_1\Big|\phi_2\Big\rangle \tag{11}$$

2 Problem 2: Dynamical Quantity F and Time-Dependent Schrödinger Equation (10 points)

2.0.1 Question

Consider a dynamical quantity F given by the expectation value of the operator $\hat{F}$:

$$\langle F\rangle = \int_{-\infty}^{\infty} \Psi^*(x,y,z,t)\hat{F}\Psi(x,y,z,t)\,d\tau$$

Use the time-dependent Schrödinger equation and the turnover rule to prove that:

$$\frac{d\langle F\rangle}{dt} = \frac{i}{\hbar}\int_{-\infty}^{\infty} \Psi^*(x,y,z,t)(\hat{H}\hat{F} - \hat{F}\hat{H})\Psi(x,y,z,t)\,d\tau$$

where $\hat{H}$ is the Hamiltonian operator and $\hbar$ is Planck's constant divided by 2π.

2.0.2 Answer

We start by considering:

$$\frac{d\langle F\rangle}{dt} = \frac{d}{dt}\int_{-\infty}^{\infty} \Psi^*(x,y,z,t)\hat{F}\Psi(x,y,z,t)\,d\tau = \int_{-\infty}^{\infty} \frac{\partial}{\partial t}\Big(\Psi^*(x,y,z,t)\hat{F}\Psi(x,y,z,t)\Big)\,d\tau \tag{12}$$

We can distribute the deferential:

$$= \int_{-\infty}^{\infty}\left(\frac{\partial\Psi^*(x,y,z,t)}{\partial t}\hat{F}\Psi(x,y,z,t) + \Psi^*(x,y,z,t)\frac{\partial\hat{F}}{\partial t}\Psi(x,y,z,t) + \Psi^*(x,y,z,t)\hat{F}\frac{\partial\Psi(x,y,z,t)}{\partial t}\right)\,d\tau \tag{13}$$

Now, the time dependent Schrödinger equation tells us that:

$$i\hbar\frac{\partial\Psi(x,y,z,t)}{\partial t} = \hat{H}\Psi(x,y,z,t) \tag{14}$$

and taking the complex conjugate of both sides gives us:

$$-i\hbar\frac{\partial\Psi^*(x,y,z,t)}{\partial t} = \Psi^*(x,y,z,t)\hat{H} \tag{15}$$

We can substitute this in and use the fact that F should be time independent:

$$= \int_{-\infty}^{\infty}\frac{i}{\hbar}\Big(\Psi^*(x,y,z,t)\hat{H}\hat{F}\Psi(x,y,z,t) - \Psi^*(x,y,z,t)\hat{F}\hat{H}\Psi(x,y,z,t)\Big)\,d\tau \tag{16}$$

So, we have arrived at the desired versal of:

$$= \frac{i}{\hbar}\int_{-\infty}^{\infty}\Psi^*(x,y,z,t)(\hat{H}\hat{F} - \hat{F}\hat{H})\Psi(x,y,z,t)\,d\tau \tag{17}$$

3 Problem 3: Orbital Angular Momentum Operators and Commutators (10 points)

3.0.1 Question

Use the definitions of the orbital angular momentum operators $\hat{L}_x$, $\hat{L}_y$, and $\hat{L}_z$ to derive the following commutators:

$$[\hat{L}_x, \hat{L}_y] = i\hbar\hat{L}_z$$
$$[\hat{L}_y, \hat{L}_z] = i\hbar\hat{L}_x$$
$$[\hat{L}_z, \hat{L}_x] = i\hbar\hat{L}_y$$

3.0.2 Answer

We know that we have:

$$\hat{L}_x = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y$$
$$\hat{L}_y = \hat{z}\hat{p}_x - \hat{x}\hat{p}_z$$
$$\hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x$$

So, evaluating the commutator $[\hat{L}_x, \hat{L}_y]$:

$$\begin{aligned}[\hat{L}_x, \hat{L}_y] &= [\hat{y}\hat{p}_z - \hat{z}\hat{p}_y, \hat{z}\hat{p}_x - \hat{x}\hat{p}_z] \\ &= [\hat{y}\hat{p}_z, \hat{z}\hat{p}_x] - [\hat{y}\hat{p}_z, \hat{x}\hat{p}_z] - [\hat{z}\hat{p}_y, \hat{z}\hat{p}_x] + [\hat{z}\hat{p}_y, \hat{x}\hat{p}_z]\end{aligned} \tag{18}$$

Sense the only terms that fail to commute are x with p_x, y with p_y, and z with p_z, the middle to terms drop out, leaving:

$$= [\hat{y}\hat{p}_z, \hat{z}\hat{p}_x] + [\hat{z}\hat{p}_y, \hat{x}\hat{p}_z] = \hat{y}\hat{p}_x[\hat{p}_z, \hat{z}] + \hat{x}\hat{p}_y[\hat{z}, \hat{p}_z] \tag{19}$$

Now we can use the canonical commutation relation $[\hat{z}, \hat{p}_z] = i\hbar$ to get:

$$= \hat{y}\hat{p}_x(-i\hbar) + \hat{x}\hat{p}_y(i\hbar) = i\hbar(\hat{x}\hat{p}_y - \hat{y}\hat{p}_x) = i\hbar\hat{L}_z \tag{20}$$

Cyclic permutation of the indices gets as the other commutators.

4 Problem 4: Linear Momentum Operator and Hermitian Property (10 points)

4.0.1 Question

The linear momentum operator is $\hat{p}_x = -i\hbar\frac{\partial}{\partial x}$. Use integration by parts in the following integral to prove that $\hat{p}_x$ is Hermitian (i.e., self-adjoint).

$$\int_{-\infty}^{+\infty} \left(-i\hbar\frac{\partial \phi_1}{\partial x}\right)^* \phi_2 \, dx$$

where the wavefunctions ϕ_1 and ϕ_2 vanish at $\pm\infty$.

4.0.2 Answer

To start with, we will move the constant terms out in front of the integral:

$$\begin{aligned}\int_{-\infty}^{+\infty} \left(-i\hbar\frac{\partial \phi_1}{\partial x}\right)^* \phi_2 \, dx &= (-i\hbar)^* \int_{-\infty}^{+\infty} \left(\frac{\partial \phi_1}{\partial x}\right)^* \phi_2 \, dx \\ &= i\hbar \int_{-\infty}^{+\infty} \left(\frac{\partial \phi_1}{\partial x}\right)^* \phi_2 \, dx\end{aligned} \tag{21}$$

Choosing $u = \phi_2$ and $dv = \left(\frac{\partial \phi_1}{\partial x}\right)^*$, we have $du = \frac{\partial \phi_2}{\partial x}$ and $v = \phi_1^*$. So, we have:

$$\begin{aligned} \int_{-\infty}^{+\infty} \left(-i\hbar \frac{\partial \phi_1}{\partial x}\right)^* \phi_2 \, dx &= i\hbar \left(\phi_1^* \phi_2\right)_{-\infty}^{+\infty} - i\hbar \int_{-\infty}^{+\infty} \phi_1^* \frac{\partial \phi_2}{\partial x} \, dx \\ &= 0 + \int_{-\infty}^{+\infty} \phi_1^* \left(-i\hbar \frac{\partial \phi_2}{\partial x}\right) dx \end{aligned} \tag{22}$$

So, indeed we have shown that

$$\langle \phi_1 | \, \hat{p}_x \, |\phi_2\rangle = \langle \phi_2 | \, \hat{p}_x \, |\phi_1\rangle^* \tag{23}$$

with equation 5 on the left and the integral in the question on the right. $\hat{p}_x$ being the transpose contract of itself is the definition of Hermiticity.

5 problem 5

5.1 Answer

$$\frac{dN_k}{dt} = AN_l + BN_l \rho(v_{kl}) - BN_k \rho(v_{kl}) \tag{24}$$

for the oder state, we would have:

$$\frac{dN_l}{dt} = -AN_l - BN_l \rho(v_{kl}) + BN_k \rho(v_{kl}) \tag{25}$$

5.2 Answer

We want to change equation 24 to a single variable, by substituting $N_k = N_{Total} - N_l$ into the first equation, we get:

$$\frac{dN_l}{dt} = -AN_l - BN_l \rho(v_{kl}) + B(N_{Total} - N_l)\rho(v_{kl}) \tag{26}$$

Grouping together the factors of N_l and N_{Total}, we get:

$$\frac{dN_l}{dt} = -AN_l + BN_{Total}\rho(v_{kl}) - 2BN_l \rho(v_{kl}) = BN_{Total}\rho(v_{kl}) - (A + 2B\rho(v_{kl}))N_l \tag{27}$$

This reminds us of $\frac{dx}{dt} + \alpha(t)x = \beta(t)$, so we can use the integrating factor method with $\alpha(t) = A + 2B\rho(v_{kl})$ and $\beta(t) = BN_{Total}\rho(v_{kl})$ with the integrating factor $\mu(t) = e^{\int \alpha dt} = e^{(A+2B\rho(v_{kl}))t}$ to get:

$$\frac{d}{dt}(N_l e^{(A+2B\rho(v_{kl}))t}) = BN_{Total}\rho(v_{kl}) e^{(A+2B\rho(v_{kl}))t} \tag{28}$$

Now, we can integrate on both sides with respect to t:

$$N_l e^{(A+2B\rho(v_{kl}))t} = \int BN_{Total}\rho(v_{kl}) e^{(A+2B\rho(v_{kl}))t} dt = \frac{BN_{Total}\rho(v_{kl})}{A + 2B\rho(v_{kl})} e^{(A+2B\rho(v_{kl}))t} + C \tag{29}$$

Solving for N_l:

$$N_l = \frac{BN_{Total}\rho(v_{kl})}{A + 2B\rho(v_{kl})} + Ce^{-(A+2B\rho(v_{kl}))t} \tag{30}$$

Now, we can use the initial condition $N_l(0) = 0$ to solve for C:

$$0 = \frac{BN_{Total}\rho(v_{kl})}{A + 2B\rho(v_{kl})} + C \tag{31}$$

Rearranging, we get:

$$C = -\frac{BN_{Total}\rho(v_{kl})}{A + 2B\rho(v_{kl})} \tag{32}$$

So, we have:

$$N_l(t) = \frac{BN_{Total}\rho(v_{kl})}{A + 2B\rho(v_{kl})}\left(1 - e^{-(A+2B\rho(v_{kl}))t}\right) \tag{33}$$

Since $N_k = N_{Total} - N_l$, we have:

$$N_k(t) = N_{Total} - \frac{BN_{Total}\rho(v_{kl})}{A + 2B\rho(v_{kl})}\left(1 - e^{-(A+2B\rho(v_{kl}))t}\right) \tag{34}$$

5.3 Answer

As $t \to \infty$, we have:

$$N_l(t) \to \frac{BN_{Total}\rho(v_{kl})}{A + 2B\rho(v_{kl})} \tag{35}$$

and

$$N_k(t) \to N_{Total} - \frac{BN_{Total}\rho(v_{kl})}{A + 2B\rho(v_{kl})} = N_{Total}\left(1 - \frac{B\rho(v_{kl})}{A + 2B\rho(v_{kl})}\right) \tag{36}$$

5.4 Answer

Consider the limit as $t \to \infty$ of $\frac{N_l(t)}{N_{Total}}$:

$$\frac{N_l(t)}{N_{Total}} \to \frac{B\rho(v_{kl})}{A + 2B\rho(v_{kl})} \tag{37}$$

No matter how you increase $\rho(v_{kl})$, the fraction will never be greater than $\frac{B}{2B} = \frac{1}{2}$. So, the fraction of atoms in the excited state will never be greater than $\frac{1}{2}$. So the answer is no.

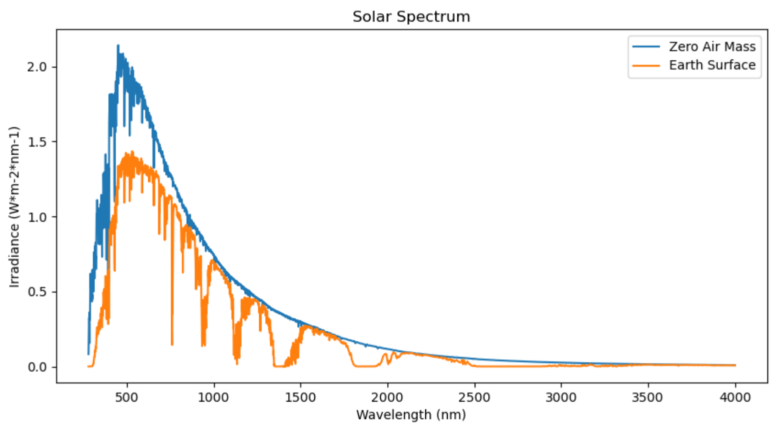
6 Problem 6: Spectral Analysis of Sunlight

6.0.1 Question (a)

Make an overlay plot of intensity vs. wavelength of the two spectra using the units provided in the file.

6.0.2 Answer (a)

To plot the overlay of the two spectra, I used some Python code with pandas and matplotlib:



6.0.3 Question (b)

What fraction of the light power at the Earth's surface is in the visible spectral region (400-700 nm)?

6.0.4 Answer (b)

Using my python script, I found this to be: 0.4233848887511344

6.0.5 Question (c)

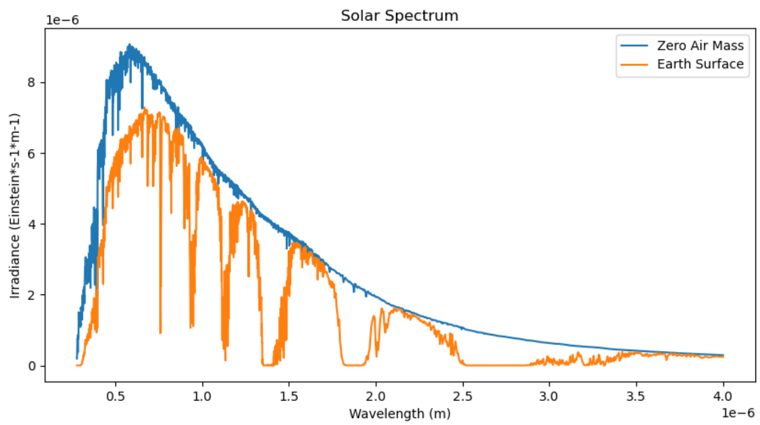
Use Planck's equation for the energy of a photon ($E = hv$) to make a new overlay plot of photon flux vs. wavelength of the two spectra using flux units of Einsteins per second per square meter per nanometer (Einsteins^{-1}m^{-2}nm^{-1}). The Einstein unit is defined to be 1 mole of photons.

6.0.6 Answer (c)

We need to formulate an equation that will let us convert from Watts per square meter per nanometer to Einsteins^{-1}m^{-2}nm^{-1}. We know that:

$$E = hv = \frac{hc}{\lambda} \tag{38}$$

So, we can use this to get the energy of a photon at a given wavelength.



6.0.7 Question (d)

What fraction of the photons reaching the Earth's surface is in the visible spectral region (400-700 nm)?

6.0.8 Answer (d)

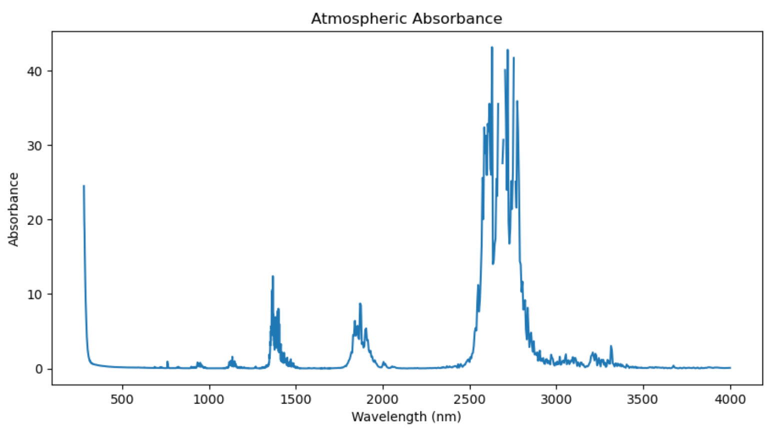
To find the fraction of photons in the visible region, we perform the calculation using a similar python script: 0.29372284127095055

6.0.9 Question (e)

The light absorbance of a sample is defined by the equation: $\text{Abs} = -\log_{10}(\frac{I}{I_0})$, where I_0 is the intensity of light incident on the sample and I is the intensity of transmitted through the sample. Use the data in the Excel file to plot the absorbance as a function of wavelength for the atmosphere.

6.0.10 Answer (e)

The absorbance of the atmosphere is plotted as a function of wavelength:


Atmospheric Absorbance
Absorbance
Wavelength (nm)
0
10
20
30
40
500
1000
1500
2000
2500
3000
3500
4000