Practice

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1 Practice Problems

1.0.1 1. You're my density

The Density Matrix provides an alternative way to specify the state of a quantum system, and can be defined as

$$\mathbf{D} = \Psi\Psi^* \tag{1}$$

where Ψ is the wavefunction and Ψ^* is its complex conjugate. Two practically compute the density matrix, a basis is chosen to expand the wavefunction in, and the densitry matrix elements are defined in terms of the expansion coefficients. That is, for the following expansion of the wavefunction in the basis of energy eigenstates,

$$\Psi(x) = \sum_i^N c_i \psi_i(x), \tag{2}$$

the density matrix elements are given by

$$D_{ij} = c_i c_j^*, \tag{3}$$

where c_j^* is the complex conjugate of the expansion coefficient c_j.

(a) Consider an electron in a box of length $L = 10$ atomic units whose wavefunction is given by

$$\Psi(x) = 1\,\psi_1(x) + 0\,\psi_2(x), \tag{4}$$

write the $2x2$ Density matrix for this system.

We can also write the Hamiltonian as a matrix ($\mathbf{H}$) in the same basis in which we wrote the Density Matrix, and if we do, we can compute the energy expectation value in the following way:

$$\langle E \rangle = \text{Tr}\,(\mathbf{HD}) \tag{5}$$

where the trace operationr (Tr) simply sums up the diagonal elements that results from the multiplication of $\mathbf{H}$ and $\mathbf{D}$.

(b) If the elements of the Hamiltonian matrix are given by

$$H_{ij} = \int_0^L \psi_i^*(x)\hat{H}\psi_j(x)dx, \tag{6}$$

compute the energy expectation value of the density matrix you calculated above.

(c) Consider the wavefunction given by

$$\Psi(x) = \sqrt{\frac{2}{3}}\psi_1(x) + \sqrt{\frac{1}{3}}\psi_2(x), \tag{7}$$

write the corresponding density matrix and compute the energy expectation value using the trace relation given above.

2 Delta Force Part 1: Exceeding Expectations

Imagine a delta function potential is introduced in the middle of the box described in **You're my density** such that the new Hamiltonian operator can be written as (in atomic units):

$$\hat{H} = -\frac{1}{2}\frac{d^2}{dx^2} + \delta(x-5). \tag{8}$$

(a) Re-compute the Hamiltonian matrix in the basis of the first two energy eigenfunctions of the particle-in-a-box using the Hamiltonian that includes the delta function potential.

(b) Using this Hamiltonian matrix, re-compute the two energy expectation values corresponding to the two density matrices you computed in (b) and (c) of **You're my density**. Has the energy expectation value increased or decreased with inclusion of the delta function potential?

Hint : The delta function has a very simple definition in terms of its integration with any other function; nameley,

$$f(x_0) = \int_{-\infty}^{\infty} f(x)\delta(x-x_0)dx. \tag{9}$$

3 Who's in Liouville

The analog of the time-dependent Schrodinger equation for the density matrix is called the Liouville equation, and has the form

$$\frac{d}{dt}\mathbf{D} = \frac{-i}{\hbar}[\mathbf{H},\mathbf{D}], \tag{10}$$

where $[\mathbf{H},\mathbf{D}] = \mathbf{HD} - \mathbf{DH}$ is known as a commutator of the Hamiltonian and Density matrices.

Derive the Liouvlle equation from the time-dependent Schrodinger equation and the definition of the Density Matrix given above.

Hint : The equation of motion of the complex conjugate of the wavefunction can be written as

$$-i\hbar\frac{d}{dt}\Psi^* = \Psi^*\hat{H}. \tag{11}$$

4 Delta Force Part 2: Not so Giant-Steps forward

Using the Hamiltonian matrix you computed in **Delta Force Part 1**, compute the time-derivative of the density matrices you computed in part (a) and (c) of **You're my density**. Based on this derivative, do you expect the diagonal elements of the density matrices to change with time, the off-diagonal elements, or both?

You can solve this problem by hand, but a better strategy would be to write a simple python program to do it.