

## Worksheet 5.

1. Write a Slater determinant of orbitals that is appropriate for the *ground* state of the Boron atom. Use the long form of the Slater determinant, writing out all the rows and columns.

2. **Properties of the Second Derivative Operator.**

In this problem, you will derive some properties of the second derivative operator,

$$\left\langle \Psi(x) \left| \frac{d^2}{dx^2} \right| \Psi(x) \right\rangle$$

- 2a. Explicitly show that the second derivative operator is Hermitian.
- 2b. Explicitly show that the second derivative operator is negative semidefinite. That is, show that for any wavefunction,  $\Psi(x)$ ,

$$\left\langle \Psi(x) \left| \frac{d^2}{dx^2} \right| \Psi(x) \right\rangle \leq 0.$$

3. **Atomic Diffraction and Neutron Diffraction.**

Suppose we use a beam of Helium-4 atoms to image a crystal, in a manner similar to X-ray crystallography. Assume that the  ${}^4_2\text{He}$  atoms are in thermal equilibrium at temperature  $T$ . From fundamental thermodynamics, we know that the kinetic energy of the Helium atoms is

$$\text{kinetic energy} = \frac{3}{2} k_B T \quad (1)$$

where  $k_B$  is Boltzmann's constant. Suppose that the substance we want to diffract the Helium atoms from crystallizes in a simple cubic lattice with lattice constant (i.e., nearest-neighbor distance)  $a = 3.0 \cdot 10^{-10} \text{ m}$ .

- 3a. At what temperature would diffraction of the  ${}^4_2\text{He}$  atoms become appreciable?
- 3b. Suppose we use thermal neutrons, instead of  ${}^4_2\text{He}$  to diffract off the crystal. **Would the optimal temperature of the neutrons be smaller or larger than that of the Helium atoms in part (a)?**
- (i)  $T_{\text{neutrons}} > T_{\text{Helium}}$                       (ii)  $T_{\text{neutrons}} < T_{\text{Helium}}$
- 3c. Suppose we now decide to diffract  ${}^4_2\text{He}$  from a cubic lattice with a slightly smaller lattice constant,  $a = 2.8 \cdot 10^{-10} \text{ m}$ . **Should the temperature of the Helium atom beam be increased or decreased in order to optimize diffraction.**
- (i)  $T_{\text{He for } .28 \text{ nm}} > T_{\text{He for } .20 \text{ nm}}$  (increase T)      (ii)  $T_{\text{He for } .28 \text{ nm}} < T_{\text{He for } .20 \text{ nm}}$  (decrease T)

**4. Mathematical results related to infinitesimal unitary transformations.**

Let  $\hat{C}(\tau)$  be a time-independent Hermitian operator. Let  $\Psi_k(\tau)$  denote the eigenfunctions of the Hamiltonian,  $\hat{H}(\tau)$ . Denote the ground-state wavefunction as  $\Psi_0(\tau)$ .

- 4a. Show that for any eigenfunction of the Hamiltonian, the following expectation value is zero:**

$$\left\langle \Psi_k \left| \left[ \hat{H}, \hat{C} \right] \right| \Psi_k \right\rangle = 0$$

- 4b. Show that the expectation value of the following double-commutator is always greater than or equal to zero for the ground-state wavefunction,**

$$\left\langle \Psi_0 \left| \left[ \hat{C}, \left[ \hat{H}, \hat{C} \right] \right] \right| \Psi_0 \right\rangle \geq 0$$

- 4c.** The results in problem #6 are key results associated with the theory of infinitesimal unitary transformations. The theory of infinitesimal unitary transformations describes, among other things, how wavefunctions change in time, and was the key mathematical concept behind Julian Schwinger's development of quantum field theory, for which he shared the 1965 Nobel Prize and became justly famous. The key idea here is that the following operator,

$$\hat{U}_\varepsilon = \hat{I} + i\varepsilon\hat{C}$$

is an infinitesimal unitary transformation, where  $\hat{I}$  is the identity operator (i.e., “multiply by one”). Here  $\varepsilon$  is a very small (“infinitesimal”) real number.

Using equations, explain why  $\hat{U}_\varepsilon$  can be interpreted as an “infinitesimal unitary transformation” if  $\hat{C}$  is a Hermitian operator, but cannot be interpreted as an “infinitesimal unitary transformation” if  $\hat{C}$  is not Hermitian. (5 points) (This requires you to remember that a unitary transformation/matrix/operator is defined by the fact that its Hermitian conjugate is equal to its inverse.)

**5. Some physicists speculate that Planck's constant might not really be constant but, instead, vary slightly in space. A physicist speculates that Planck's constant on the moon is slightly smaller than Planck's constant on earth. We decide to test this hypothesis using the one-dimensional particle in a box. Which of the following observations are would support this hypothesis.**

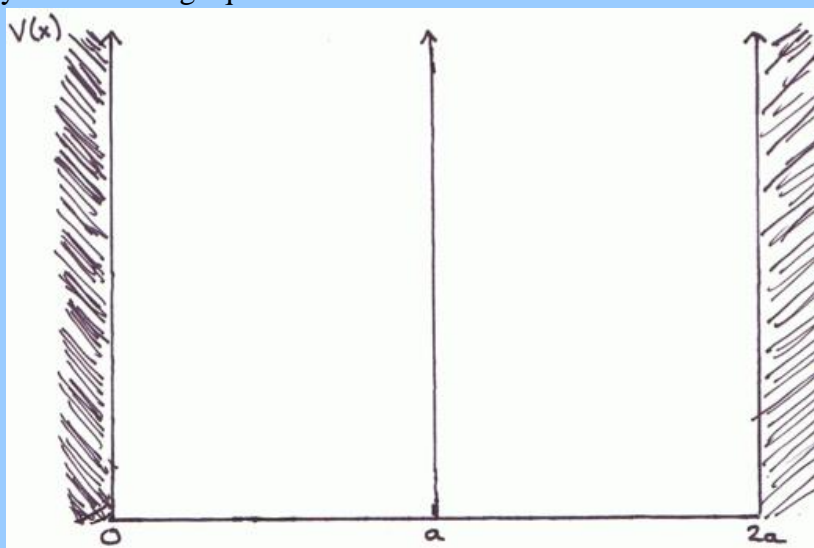
- (a) the zero-point energy of the “moon box” is less than that of the “earth box.”
- (b) the zero-point energy of the “moon box” is equal to that of the “earth box.”
- (c) the zero-point energy of the “moon box” is greater than that of the “earth box.”
- (d) the average position of the particle is further from the edges of the “moon box” than the “earth box.”
- (d) the average position of the particle is closer to the edges of the “moon box” than the “earth box.”
- (e) the average position of the particle in the “moon box” than the “earth box” is the same.

6. Write down the time-dependent Schrodinger equation.
7. Assume the Hamiltonian is time-independent, and that it has eigenfunctions  $\hat{H}\psi_k(\mathbf{r}) = E_k\psi_k(\mathbf{r})$ . Use separation of variables on the time-dependent Schrödinger equation to solve for the space+time-dependent wavefunction,  $\Psi(\mathbf{r}, t)$ .

The following text refers to problems 8-10.

Consider an electron confined to two one-dimensional boxes with infinitely repulsive sides. The two boxes are adjacent to each other but separated by an infinite barrier, as shown in the following figure and encapsulated by the following equation:

$$V(x) = \begin{cases} +\infty & x \leq 0 \\ 0 & 0 < x < a \\ +\infty & x = a \\ 0 & a < x < 2a \\ +\infty & x \geq 2a \end{cases}$$



8. The system is prepared in its ground state and then its absorption spectrum is taken. The largest-wavelength absorption that is observed has wavelength 1000 nm. **How wide are the boxes? (I.e., what is the value of  $a$ ?)**
9. **What is the ground state energy of this system?**
10. An experiment reveals that the system has a 90% chance of being observed in the first box and a 10% chance of being observed in the second box. **Write TWO wavefunctions, which differ from each other by more than a constant factor, that are consistent with this observation.**