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## 3.23 Electrical, Optical, and Magnetic Properties of Materials

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# Quantum Mechanics - exercise sheet 2

Nicolas Poilvert

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## 1

In order to find the quantum mechanical expression for a physical observable that has a classical analog, we use the **Canonical quantization rules**. Those rules state that if a classical observable  $O(\vec{r}, \vec{p})$  is a function of the position  $\vec{r}$  and the momentum  $\vec{p}$ , then to obtain the quantum analog, we must replace the position by the position observable  $\hat{r}$  and the momentum by the momentum observable  $\frac{\hbar}{i}\vec{\nabla}$ . Therefore we obtain a differential operator  $\hat{O}$  that can act on a wavefunction.

1) The classical kinetic energy is a function of position and momentum, because  $T(\vec{r}, \vec{p}) = \frac{p^2}{2m}$ . Using the quantization rules can you express the quantum kinetic energy operator?

2) In classical mechanics, the angular momentum is a function of position and momentum, because  $L(\vec{r}, \vec{p}) = \vec{r} \times \vec{p}$ . Using the quantization rules find the expression of the quantum angular momentum operator.

3) The electrical current generated by the motion of an electron is a classical observable, because  $\vec{j} = -e\vec{v} = -\frac{e}{m}\vec{p}$ . What is the expression of the quantum electrical current operator?

## 2

We have seen in the lectures that every physical observable has a representation in quantum mechanics. Indeed an observable is represented by a Hermitian operator. One of the reasons why we represent observable by Hermitian operators in quantum mechanics is because those operators have the great quality of having only **real eigenvalues**. This is important because the eigenvalues of an observable are the **only possible outcomes** of experiments measuring the associated physical quantity.

1) Let  $\hat{O}$  be an observable. That observable is then an hermitian operator. What does it mean to be hermitian for an operator? (Use both Dirac's "bra-ket" notation and wavefunctions to express hermiticity).

2)  $\hat{O}$  being an Hermitian operator, it has a complete set of eigenvectors  $\psi_n(x)$  and also a set of eigenvalues  $a_n$ , such that  $\hat{O}\psi_n(x) = a_n\psi_n(x)$  for all n. Using the above property of hermiticity, can you prove that any eigenvalue  $a_n$  is necessarily **real**?

### 3

We have seen in class that the set of all the eigenvectors of an operator is orthonormal. To verify this on an example, let's consider the set of all the eigenfunctions of the total energy operator for an electron in a one dimensional infinite well. The eigenfunctions are:

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin(n\pi \frac{x}{a}) \text{ with } n \text{ any positive integer and } a \text{ the length of the well}$$

- 1) Can you verify that each of those functions is normalized?
- 2) Let's take two strictly positive integers  $n$  and  $m$ . Prove that  $\psi_n(x)$  and  $\psi_m(x)$  are orthogonal.

### 4

The momentum operator along  $x$  is given by  $p_x = \frac{\hbar}{i} \frac{\partial}{\partial x}$  and the position operator is given by  $x$ . Let's consider a wavefunction  $\psi(x, y, z)$ .

- 1) What is the result of applying  $x p_x - p_x x$  onto the wavefunction  $\psi(x, y, z)$ ?
- 2) What can you conclude about the commutator  $[x, p_x]$ ?
- 3) What is the result of applying  $y p_x - p_x y$  onto the wavefunction  $\psi(x, y, z)$ ?
- 4) What can you say about the commutator  $[y, p_x]$ ?

### 5

In class, we saw that the projection of the angular momentum along the  $z$  axis,  $L_z$ , had a fairly simple expression in spherical coordinates:  $L_z = \frac{\hbar}{i} \frac{\partial}{\partial \phi}$ . We also know the expression of  $L_z$  in cartesian coordinates:  $L_z = \frac{\hbar}{i} \left( x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right)$ .

1) What are the expressions of  $x$ ,  $y$  and  $z$  in terms of spherical coordinates  $r$ ,  $\theta$  and  $\phi$ ?

2) Can you express the partial derivative with respect to  $x$ ,  $\frac{\partial}{\partial x}$ , in terms of partial derivatives with respect to  $r$ ,  $\theta$  and  $\phi$  and the spherical coordinates themselves using the **chain rule**? (there must remain no  $x$ ,  $y$  and  $z$  in the expression for  $\frac{\partial}{\partial x}$ )

The chain rule in math:

The chain rule states that if  $x$  is a function of  $u$ ,  $v$  and  $w$  ( $x(u, v, w)$ ), then the partial derivative with respect to  $x$  can be expressed as a sum of terms each involving a partial derivative with respect to one of the variables  $u$ ,  $v$  and  $w$ :

$$\frac{\partial}{\partial x} = \frac{\partial}{\partial u} * \frac{\partial u}{\partial x} + \frac{\partial}{\partial v} * \frac{\partial v}{\partial x} + \frac{\partial}{\partial w} * \frac{\partial w}{\partial x}$$

Each of the terms  $\frac{\partial u}{\partial x}$ ,  $\frac{\partial v}{\partial x}$  and  $\frac{\partial w}{\partial x}$  can then be expressed in terms of  $u$ ,  $v$  and  $w$  because we know that  $\frac{\partial u}{\partial x} = \frac{1}{\frac{\partial x}{\partial u}}$  and that  $x$  is a function of  $u$ ,  $v$  and  $w$  (same result for  $\frac{\partial v}{\partial x}$  and  $\frac{\partial w}{\partial x}$ ).

3) In the same way express the partial derivative with respect to  $y$ ,  $\frac{\partial}{\partial y}$ , in terms of partial derivatives with respect to  $r$ ,  $\theta$  and  $\phi$  and the spherical coordinates themselves.

4) Now add all the pieces together in the cartesian expression of  $L_z$  to see that all the terms expressed in spherical coordinates "kill" each other and leaves you with  $\frac{\hbar}{i} \frac{\partial}{\partial \phi}$ .