3.23 Electrical, Optical, and Magnetic Properties of Materials
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Quantum Mechanics - exercise sheet 2, solutions

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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 $\hat{\vec{r}}$ 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 $T(\vec{r}, \vec{p}) = \frac{\vec{p}^2}{2m}$. Using the quantization rules can you express the quantum kinetic energy operator?

solution:

By plugging $\vec{\hat{p}} = \frac{\hbar}{i}\vec{\nabla}$ in $\hat{T} = \frac{\vec{p}^2}{2m}$, we find:

$$\hat{T} = -\frac{\hbar^2}{2m}\vec{\nabla} \cdot \vec{\nabla}$$

And the dot product is just $\vec{\nabla} \cdot \vec{\nabla} = \frac{\partial}{\partial x}\frac{\partial}{\partial x} + \frac{\partial}{\partial y}\frac{\partial}{\partial y} + \frac{\partial}{\partial z}\frac{\partial}{\partial z} = \vec{\nabla}^2$ which is the Laplacian.

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.

solution:

The angular momentum is given by $\vec{\hat{L}} = \vec{\hat{r}} \times \frac{\hbar}{i}\vec{\hat{\nabla}}$. For example the z component of the angular momentum is given by:

$$\hat{L}_z = \hat{x}\hat{p}_x - \hat{y}\hat{p}_y = \frac{\hbar}{i}(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x})$$

The other components are:

$$\hat{L}_x = \frac{\hbar}{i}(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y})$$

and

$$\hat{L}_y = \frac{\hbar}{i}(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z})$$

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?

solution:

With the above definition, we see that the current density is simply:

$$\vec{\hat{j}} = -\frac{e}{m}\frac{\hbar}{i}\vec{\nabla}$$

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).

solution:

Being hermitian means that, given ψ and ϕ, we have: $\left\langle \psi | \hat{O}\phi \right\rangle = \left\langle \hat{O}\psi | \phi \right\rangle$.

In terms of wavefunctions: $\int \psi^*(\vec{r})\hat{O}(\phi(\vec{r}))d\vec{r} = \int (\hat{O}\psi(\vec{r}))^*\phi(\vec{r})d\vec{r}$.

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**?

solution:

Let's consider an eigenvalue a_n and a corresponding eigenvector $|\psi_n\rangle$. Since $\hat{O}$ is hermitian, we have:

$$\left\langle \psi_n | \hat{O}\psi_n \right\rangle = \int \psi_n^*(\vec{r})\hat{O}(\psi_n(\vec{r}))d\vec{r} = \int \psi_n^*(\vec{r})a_n(\psi_n(\vec{r}))d\vec{r}$$

But since $\psi_n(\vec{r})$ is normalized, we see that the above expression leads to a_n. On the other hand because $\hat{O}$ is hermitian, the above expression must be equal to the following one:

$$\left\langle \psi_n | \hat{O}\psi_n \right\rangle = \left\langle \hat{O}\psi_n | \psi_n \right\rangle = \int (\hat{O}\psi_n(\vec{r}))^*\psi_n(\vec{r})d\vec{r} = \int (a_n\psi_n(\vec{r}))^*\psi_n(\vec{r})d\vec{r} = a_n^*$$

We can then conclude that if $\hat{O}$ is hermitian, $a_n = a_n^*$ for any eigenvalue. So **eigenvalues of hermitian operators are real numbers**.

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:

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

1) Can you verify that each of those functions is normalized?

solution:

We have $\int_0^a |\psi_n(x)|^2 dx = \int_0^a \frac{2}{a}\sin^2(n\pi\frac{x}{a})dx = \frac{2}{a}\int_0^a (\frac{1-\cos(2n\pi\frac{x}{a})}{2})dx$. In the last term the integral of the cosine function over many periods gives us zero and so the wavefunction is normalized.

2) Let's take two strictly positive integers n and m. Prove that $\psi_n(x)$ and $\psi_m(x)$ are orthogonal.

To answer this question one will need to use the following trigonometric identity: $\sin(a)\sin(b) = \frac{\cos(a-b)-\cos(a+b)}{2}$. Using this we wee that:

$$\langle\psi_n|\psi_m\rangle = \frac{2}{a}\int_0^a \sin(n\pi\frac{x}{a})\sin(m\pi\frac{x}{a})dx =$$
$$\frac{1}{a}\int(\cos((n-m)\pi\frac{x}{a}) - \cos((n+m)\pi\frac{x}{a}))dx$$

And we are left with two terms each involving an integration of a cosine function over many periods, which is zero. In the end the scalar product of ψ_n with ψ_m gives us zero and we can say that the two functions 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 $xp_x - p_x x$ onto the wavefunction $\psi(x,y,z)$?
solution:

Let's apply $xp_x - p_x x$ onto $\psi(x,y,z)$. We find $(xp_x - p_x x)\psi(x,y,z) = x\frac{\hbar}{i}\frac{\partial\psi}{\partial x} - \frac{\hbar}{i}\frac{\partial(x\psi)}{\partial x} = -\frac{\hbar}{i}\psi(x,y,z)$

2) What can you conclude about the commutator $[x, p_x]$?
solution:

We can conclude that : $[x, p_x] = -\frac{\hbar}{i} = i\hbar$. Position along x and the x component of the momentum cannot be measured at the same time because the commutator of the two operators is not zero.

3) What is the result of applying $yp_x - p_x y$ onto the wavefunction $\psi(x,y,z)$?
solution:

In this case we see that when we derive with respect to x in the second term, we can pull out the y variable (something we could not do in question 1)). We can therefore conclude that $yp_x - p_x y$ applied to any wavefunction $\psi(x,y,z)$ gives us zero.

4) What can you say about the commutator $[y, p_x]$?
solution:

From question 3) we can conclude that : $[y, p_x] = 0$. Physically speaking this means that the position along x and the y component of the momentum **can** be measured at the same time with infinite precision (at least in principle).

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, θ and ϕ?
solution:

In general, we have:

- $x = r\sin(\theta)\cos(\phi)$

- $y = r\sin(\theta)\sin(\phi)$

- $z = r\cos(\theta)$

2) Can you express the partial derivative with respect to x, $\frac{\partial}{\partial x}$, in terms of partial derivatives with respect to r, θ and ϕ 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 $\frac{\partial w}{\partial x}$).

solution:

Using the chain rule, we can calculate $\frac{\partial}{\partial x}$:

$$\frac{\partial}{\partial x} = \frac{\partial}{\partial r} * \frac{\partial r}{\partial x} + \frac{\partial}{\partial \theta} * \frac{\partial \theta}{\partial x} + \frac{\partial}{\partial \phi} * \frac{\partial \phi}{\partial x}$$

Now we need to calculate $\frac{\partial r}{\partial x}$, $\frac{\partial \theta}{\partial x}$ and $\frac{\partial \phi}{\partial x}$. To do this we will express r, θ and ϕ in terms of x, y and z and partially differentiate with respect to x. We know that $r^2 = x^2 + y^2 + z^2$, $x^2 + y^2 = r^2\sin^2(\theta)$ and $\tan(\phi) = \frac{y}{x}$ (you can easily check that). So if we differentiate r^2 with respect to x and $x^2 + y^2 + z^2$ with respect to x and equate those two expressions we find: $2r\frac{\partial r}{\partial x}dx = 2xdx$, which leads us to : $\frac{\partial r}{\partial x} = \frac{x}{r} = \sin(\theta)\cos(\phi)$. If we follow similar steps with $x^2 + y^2 = r^2\sin^2(\theta)$ and $\tan(\phi) = \frac{y}{x}$, we can easily find the following results : $\frac{\partial \theta}{\partial x} = \frac{\cos(\phi)}{r\cos(\theta)}$ and $\frac{\partial \phi}{\partial x} = -\frac{\sin(\phi)}{r\sin(\theta)}$. All in all, we end up with:

$$\frac{\partial}{\partial x} = \frac{\partial}{\partial r} * \sin(\theta)\cos(\phi) + \frac{\partial}{\partial \theta} * \frac{\cos(\phi)}{r\cos(\theta)} + \frac{\partial}{\partial \phi} * \left(-\frac{\sin(\phi)}{r\sin(\theta)}\right)$$

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, θ and ϕ and the spherical coordinates themselves.

solution:

Using the exact same steps but differentiating with respect to y, we find:

$$\frac{\partial}{\partial y} = \frac{\partial}{\partial r} * \sin(\theta)\sin(\phi) + \frac{\partial}{\partial \theta} * \frac{\sin(\phi)}{r\cos(\theta)} + \frac{\partial}{\partial \phi} * \frac{\cos(\phi)}{r\sin(\theta)}$$

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 $\frac{\hbar}{i}\frac{\partial}{\partial \phi}$.

By definition $\hat{L}_z$ is $\frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$. Given the expressions for x, y, $\frac{\partial}{\partial x}$ and $\frac{\partial}{\partial y}$ in terms of spherical coordinates, you can easily check that the partial derivatives with respect to r and θ "kill" each other and one ends up with the remaining term $\frac{\hbar}{i}\frac{\partial}{\partial \phi}$!