3.23 Electrical, Optical, and Magnetic Properties of Materials
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Quantum Mechanics - exercice sheet 1, solution

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By definition, the **De Broglie** formula is $\lambda = \frac{h}{p}$, where h is the Planck constant and p is the momentum's magnitude. We also know from classical mechanics that the momentum is related the the velocity by $p = mv$, where m is the mass of the particle. We can then conclude that the **De Broglie** wavelength is given by:

$$\lambda = \frac{h}{\sqrt{3mk_BT}}$$

If M is the molar mass, the mass of a single atom is $m = \frac{M}{N_A}$, where N_A is the Avogadro number. We find that:

- $\lambda_{\text{He}}^{100K} \approx 1.26\text{Å}$ and $\lambda_{\text{He}}^{500K} \approx 0.56\text{Å}$
- $\lambda_{\text{Ar}}^{100K} \approx 0.40\text{Å}$ and $\lambda_{\text{Ar}}^{500K} \approx 0.18\text{Å}$

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Using the **De Broglie** formula, we easily find that:

$$\lambda = \frac{h}{mv} \Longrightarrow v = \frac{h}{m\lambda}$$

By plugging in the values for the mass of the electron and the typical bond length for λ, we find:

$$v \approx 4.8 * 10^6\text{m.s}^{-1} \text{ which is about } 1.6\% \text{ of the speed of light!}$$

3

According to the probabilistic interpretation of the wavefunction in Quantum Mechanics, we know that if the wavefunction of any system is given by $\psi(\vec{r}, t)$, then the probability to find the system in a small volume $d^3\vec{r}$ around position $\vec{r}$ at time t is:

$$P(\vec{r}, t)d^3\vec{r} = |\psi(\vec{r}, t)|^2 d^3\vec{r}$$

Now if the expression for the wavefunction is $\psi(\vec{r}, t) = \phi(x)e^{-\frac{iEt}{\hbar}}$ (here we deal with a one dimensional system in which $\vec{r}$ is replaced by x), then we see that $P(\vec{r}, t)$ is given by $|\phi(x)|^2$, because $|e^{-\frac{iEt}{\hbar}}|^2 = 1$. From this result we can then conclude that $P(\vec{r}, t)$ does not depend on the time t. This is why we say that wavefunctions like $\psi(x, t) = \phi(x)e^{-\frac{iEt}{\hbar}}$ represents "standing waves". In the litterature, you will also see "stationnary states" to describe "standing waves".

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In order to describe a (sinusoidal) wave travelling in the -x direction, we use the following mathematical expression:

$$\psi(x,t) = A\sin(kx + \omega t)$$

A wave represents a "perturbation" in space and time. In order to convince ourselves that this "perturbation" is indeed travelling in the -x direction, we will "follow" a plane of constant perturbation, i.e we will set $\psi(x,t)$ to a given value ψ_0. Given the mathematical expression for $\psi(x,t)$, we see that setting $\psi(x,t)$ to a constant is equivalent to setting the phase of the wave $(kx + \omega t)$ to a given constant. Now if $kx + \omega t = c_0$ =constant for all x and t, then we can write:

$$x = \frac{-\omega t + c_0}{k}$$

which shows us that x is decreasing with time. Hence the wave travells "to the left", i.e in the -x direction.

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Let's consider the set of wavefunctions $\psi_1(x), \psi_2(x), ..., \psi_n(x)$. One says that the wavefunctions in the set are **orthogonal** to each other **when** for any indices i and j in $1, 2, 3, ..., n$, we have the following result:

$$\int \psi_i^*(x)\psi_j(x)dx = \delta_{ij}$$

where δ_{ij} is one only if $i = j$ and zero otherwise.

A wavefunction $\psi(x)$ is **normalized** if we have:

$$\int \psi^*(x)\psi(x)dx = \int |\psi(x)|^2 dx = 1$$

We say that a set of wavefunctions $\psi_1(x), \psi_2(x), ..., \psi_n(x)$ is **complete**, when **any wavefunction** $\psi(x)$ can be expanded as a linear combinaison of the basis functions in the set. Mathematically, we can write any wavefunction as a sum:

$$\psi(x) = \sum_{j=1}^{n} c_j \psi_j(x)$$

where the $\psi_j(x)$ are the wavefunctions belonging to the **complete set** and the c_j's are complex numbers.

6

If we derive $\sin(\phi)\cos(\phi)$ with respect to ϕ, we find $\cos^2(\phi) - \sin^2(\phi) = \cos(2\phi)$ which is not equal to a constant time $\sin(\phi)\cos(\phi)$, so $\sin(\phi)\cos(\phi)$ is **not** an eigenfunction of the operator $\frac{\partial}{\partial\phi}$.

We have $\frac{1}{x}\frac{d}{dx}(e^{-x^2/3}) = \frac{1}{x}(-\frac{2x}{3})e^{-x^2/3} = (-\frac{2}{3})e^{-x^2/3}$. We then see that $\frac{1}{x}\frac{d}{dx}$ applied to the wavefunction $e^{-x^2/3}$ gives us $-\frac{2}{3}$ times **the same** wavefunction. We can then conclude that $e^{-x^2/3}$ **is** an eigenfunction of $\frac{1}{x}\frac{d}{dx}$ for the eigenvalue $-\frac{2}{3}$.

Again we have $\left[x\frac{\partial}{\partial x}+y\frac{\partial}{\partial y}\right]xy = x\frac{\partial(xy)}{\partial x}+y\frac{\partial(xy)}{\partial y} = xy+yx = 2xy$. We conclude that xy is an eigenfunction of $x\frac{\partial}{\partial x}+y\frac{\partial}{\partial y}$ for the eigenvalue 2.

In this case we have, $\left[\frac{1}{\sin(\theta)}\frac{d}{d\theta}(\sin(\theta)\frac{d}{d\theta})\right](3\cos(\theta)^2-1) = \frac{1}{\sin(\theta)}\frac{d}{d\theta}(\sin(\theta)\frac{d(3\cos(\theta)^2-1)}{d\theta}) = \frac{1}{\sin(\theta)}\frac{d}{d\theta}(\sin(\theta)(-6\sin(\theta)\cos(\theta))) = \frac{-6}{\sin(\theta)}\frac{d}{d\theta}(\cos(\theta)\sin(\theta)^2) = \frac{-6}{\sin(\theta)}(-\sin(\theta)^3 + 2\cos(\theta)^2\sin(\theta)) = -6(3\cos(\theta)^2-1)$. Hence $3\cos(\theta)^2-1$ **is** an eigenfunction of $\frac{1}{\sin(\theta)}\frac{d}{d\theta}(\sin(\theta)\frac{d}{d\theta})$ for the eigenvalue -6.

The last one is easy. Indeed $\frac{d}{dx}(x^2) = 2x$ which is not a number times x^2, so x^2 **is not** an eigenfunction of $\frac{d}{dx}$.

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- $ae^{-3x}+be^{-3ix}$ is **not** an eigenfunction of $\frac{d}{dx}$ because $\frac{d}{dx}(ae^{-3x}+be^{-3ix}) = -3(ae^{-3x}+ibe^{-3ix}) \neq \text{constant} * (ae^{-3x}+be^{-3ix})$
- it is quite obvious to see that $\sin^2(x)$ is **not** an eigenfunction of $\frac{d}{dx}$.
- e^{-ix} **is** clearly an eigenfunction of $\frac{d}{dx}$ for the eigenvalue $-i$
- $\cos(ax)$ is **not** an eigenvalue of $\frac{d}{dx}$ because $\frac{d}{dx}(\cos(ax)) = -a\sin(ax) \neq \text{constant} * \cos(ax)$
- At last, we see that $\frac{d}{dx}(e^{-ix^2}) = -2ixe^{-ix^2} \neq \text{constant} * e^{-ix^2}$, so e^{-ix^2} is **not** an eigenfunction of $\frac{d}{dx}$.