VARIANCE AND VECTORS: A BRIEF REVIEW

Chem 2430

For any wave function ψ (not necessarily an eigenfunction of operator $\hat{A}$),

we can complete the average using $\langle \psi | \hat{A} | \psi \rangle$

The variance is given by $\left\langle \psi \left| \left(\hat{A} - \langle \hat{A} \rangle \right)^2 \right| \psi \right\rangle$

$$= \langle \psi | \hat{A}^2 | \psi \rangle - 2 \langle \psi | \hat{A} | \psi \rangle^2 + \langle \psi | \hat{A} | \psi \rangle^2$$

$$= \langle \psi | \hat{A}^2 | \psi \rangle - \langle \hat{\psi} | \hat{A} | \psi \rangle^2$$

$$= \langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2$$

The standard deviation is $\delta_A = \Delta A = \sqrt{\langle \widehat{A}^2 \rangle - \langle \widehat{A} \rangle^2}$ = "uncertainty in A"

$$\delta_A \delta_B = \Delta A \Delta B \geq \frac{1}{2} \left| \int \psi^* \left[\hat{A}, \hat{B} \right] \psi \, d\tau \right|$$

$$= \frac{1}{2} \left| \langle \psi | \hat{A}\hat{B} - \hat{B}\hat{A} | \psi \rangle \right|$$

Roberston Equation
(proof in problem 7.58)

If $\left[\hat{A},\hat{B}\right]=0,\ \delta_A\delta_B=0$ and both ΔA and ΔB can be zero.

Suppose ψ is an eigenfunction of both $\hat{A}$ and $\hat{B}$

with $\hat{A}\psi = a\psi, \hat{B}\psi = b\psi$

$$\left\langle \psi \mid \hat{A}\hat{B}-\hat{B}\hat{A} \mid \psi \right\rangle = \left\langle \psi \mid ab-ba \mid \psi \right\rangle = 0$$

If $\hat{A}=\hat{x},\ \hat{B}=\hat{p}_x,\ \left[\hat{x},\hat{p}_x\right]=\frac{\hbar}{i}$

Then $\sigma_x\sigma_{p_x} \geq \frac{\hbar}{2}$

Heisenberg Uncertainty Principle

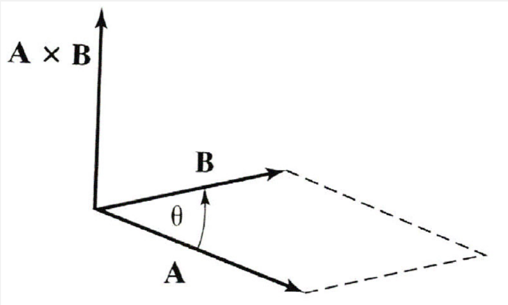
Vectors

$$\boldsymbol{A} = A_x\boldsymbol{i} + A_y\boldsymbol{j} + A_z\boldsymbol{k}$$

$$\boldsymbol{A}\cdot\boldsymbol{B} = |A||B|\cos\theta$$

$$\boldsymbol{A}\cdot\boldsymbol{A} = |\boldsymbol{A}|^2 = A_x{}^2 + A_y{}^2 + A_z{}^2$$

$$|\boldsymbol{A}x\boldsymbol{B}| = |\boldsymbol{A}||\boldsymbol{B}|\sin\theta$$



$$\boldsymbol{i}x\boldsymbol{i} = \boldsymbol{j}x\boldsymbol{j} = \boldsymbol{k}x\boldsymbol{k} = 0$$

$$\boldsymbol{i}x\boldsymbol{j} = \boldsymbol{k},\ \boldsymbol{j}x\boldsymbol{k} = \boldsymbol{i},\ \boldsymbol{k}x\boldsymbol{i} = \boldsymbol{j}$$

$$\boldsymbol{A}x\boldsymbol{B} = \left(A_yB_z - A_zB_y\right)\boldsymbol{i} + \left(A_zB_x - A_xB_z\right)\boldsymbol{j} + \left(A_xB_y - A_yB_x\right)\boldsymbol{k}$$

$$= \begin{vmatrix} \boldsymbol{i} & \boldsymbol{j} & \boldsymbol{k} \\ A_x & A_y & A_z \\ B_x & B_y & B_z \end{vmatrix}$$

$$\boldsymbol{B}x\boldsymbol{A} = -\boldsymbol{A}x\boldsymbol{B}$$

$$\nabla = \boldsymbol{i}\frac{\partial}{\partial x} + \boldsymbol{j}\frac{\partial}{\partial y} + \boldsymbol{k}\frac{\partial}{\partial z}$$

$$\hat{p} = \frac{\hbar}{i}\nabla$$

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

$$\mathrm{grad}\, g = \nabla g = \boldsymbol{i}\frac{\partial g}{\partial x} + \boldsymbol{j}\frac{\partial g}{\partial y} + \boldsymbol{k}\frac{\partial g}{\partial z}$$

This is the gradient of a scalar

$$\boldsymbol{f} = -\nabla V(x, y, z)$$

The force on an object is given by the negative of the gradient of the potential