



WFU Physics Colloquium

**TITLE:** Guided Design of Materials: from the sublime (core-shell nanoparticles) to the ridiculous (High-Entropy Alloys)\*

**SPEAKER:** Professor Duane D. Johnson  
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**TIME:** Wed, Sep. 20, 2017 at 4:00 PM

**PLACE:** George P. Williams, Jr. Lecture Hall, (Clin 101)

**ABSTRACT**

Since the Iron Age, complex alloying effects have yielded desirable and unusual behaviors whose origins were difficult to unravel. Here we address intriguing behavior from alloying that occur in metallic nanoparticles to bulk complex solid solutions.

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Commutator formalism in quantum mechanics

**Definition:**  
Given two Hermitian operators  $A$  and  $B$ , their commutator is  
 $[A, B] \equiv AB - BA$

**Theorem:**  
Given Hermitian operators  $A, B, C$  such that  
 $[A, B] = iC$ ,  
it follows that  $\Delta A \Delta B \geq \frac{1}{2} |\langle C \rangle|$

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**Note that:**

$$[A, B]^\dagger = (iC)^\dagger$$

$$(AB - BA)^\dagger = B^\dagger A^\dagger - A^\dagger B^\dagger = -iC^\dagger$$

$$= BA - AB = -iC$$

**Calculation of the variance:**

$$(\Delta A)^2 \equiv \langle \psi | (A - \langle A \rangle)^2 | \psi \rangle$$

$$= \langle (A - \langle A \rangle) \psi | (A - \langle A \rangle) \psi \rangle$$

Define  $|\psi_A\rangle \equiv (A - \langle A \rangle) \psi$   
 $|\psi_B\rangle \equiv (B - \langle B \rangle) \psi$

Similarly,  
 $(\Delta B)^2 \equiv \langle \psi | (B - \langle B \rangle)^2 | \psi \rangle$   
 $= \langle (B - \langle B \rangle) \psi | (B - \langle B \rangle) \psi \rangle$

**Schwarz inequality:**  
 $\langle \psi_A | \psi_A \rangle \langle \psi_B | \psi_B \rangle \geq |\langle \psi_A | \psi_B \rangle|^2$

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Define  $|\psi_A\rangle \equiv |(A - \langle A \rangle)\psi\rangle$  and  $|\psi_B\rangle \equiv |(B - \langle B \rangle)\psi\rangle$   
 Schwarz inequality:  
 $\langle \psi_A | \psi_A \rangle \langle \psi_B | \psi_B \rangle \geq |\langle \psi_A | \psi_B \rangle|^2$   
 $\langle \psi_A | \psi_B \rangle = \langle \psi | (A - \langle A \rangle)(B - \langle B \rangle) | \psi \rangle$   
 $(A - \langle A \rangle)(B - \langle B \rangle) = \frac{1}{2}((A - \langle A \rangle)(B - \langle B \rangle) + (B - \langle B \rangle)(A - \langle A \rangle))$   
 $\quad + \frac{1}{2}((A - \langle A \rangle)(B - \langle B \rangle) - (B - \langle B \rangle)(A - \langle A \rangle))$   
 $\quad \Rightarrow F + \frac{i}{2}C$

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$\langle \psi_A | \psi_B \rangle = \langle \psi | (A - \langle A \rangle)(B - \langle B \rangle) | \psi \rangle$   
 $\quad = \langle \psi | F | \psi \rangle + \frac{i}{2} \langle \psi | C | \psi \rangle$   
 $|\langle \psi_A | \psi_B \rangle|^2 = |\langle \psi | F | \psi \rangle|^2 + \frac{1}{4} |\langle \psi | C | \psi \rangle|^2 \geq \frac{1}{4} |\langle \psi | C | \psi \rangle|^2$   
 Putting it all together:  
 $\langle \psi_A | \psi_A \rangle \langle \psi_B | \psi_B \rangle \geq |\langle \psi_A | \psi_B \rangle|^2 \geq \frac{1}{4} |\langle \psi | C | \psi \rangle|^2$   
 $\Rightarrow (\Delta A)^2 (\Delta B)^2 \geq \frac{1}{4} |C|^2$

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$[A, B] = iC \quad \Delta A \Delta B \geq \frac{1}{2} |C|$   
 Example:  $A = X, B = P$   
 $[X, P] = i\hbar \quad \Delta X \Delta P \geq \frac{\hbar}{2}$

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**Other uses of the commutator**  
 Consider a wavefunction that solves the time-dependent Schrodinger equation:  

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi$$
 Expectation value of operator  $F$ :  

$$\langle F \rangle = \langle \psi | F | \psi \rangle$$
 Time derivative of  $\langle F \rangle$ :  

$$\frac{d\langle F \rangle}{dt} = \left\langle \frac{\partial \psi}{\partial t} \middle| F \middle| \psi \right\rangle + \langle \psi | \frac{\partial F}{\partial t} | \psi \rangle + \left\langle \psi \middle| F \left| \frac{\partial \psi}{\partial t} \right\rangle$$

$$= \frac{i}{\hbar} \langle H\psi | F | \psi \rangle + \langle \psi | \frac{\partial F}{\partial t} | \psi \rangle - \frac{i}{\hbar} \langle \psi | F | H\psi \rangle$$

$$= \frac{1}{i\hbar} \langle \psi | [F, H] | \psi \rangle + \langle \psi | \frac{\partial F}{\partial t} | \psi \rangle = \left\langle \psi \middle| \left( \frac{1}{i\hbar} [F, H] + \frac{\partial F}{\partial t} \right) \middle| \psi \right\rangle$$

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**Some other useful commutator relationships:**  
 For  $[A, [A, B]] = 0$  and  $[B, [A, B]] = 0$   

$$[A, B^n] = nB^{n-1}[A, B]$$

$$[A^n, B] = nA^{n-1}[A, B]$$
 Evaluation of the commutator  

$$[A, B]|\psi\rangle = AB|\psi\rangle - BA|\psi\rangle$$
 Example:  

$$[f(X), P]|\psi\rangle = f(X)P|\psi\rangle - Pf(X)|\psi\rangle = i\hbar \frac{\partial f}{\partial X} |\psi\rangle$$
 Note that:  $P = -i\hbar \frac{\partial}{\partial X}$

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**Angular momentum in three dimensions**  

$$L_x = YP_z - ZP_y$$

$$L_y = ZP_x - XP_z$$

$$L_z = XP_y - YP_x$$
 Consider:  

$$[L_x, Y] = [YP_z - ZP_y, Y] = -Z[P_y, Y] = i\hbar Z$$

$$[L_x, P_y] = [YP_z - ZP_y, P_y] = P_z[Y, P_y] = i\hbar P_z$$

$$[L_x, L_y] = [YP_z - ZP_y, ZP_x - XP_z] = i\hbar L_z$$
 Summary:  

$$[L_x, L_y] = i\hbar L_z \quad [L_y, L_z] = i\hbar L_x \quad [L_z, L_x] = i\hbar L_y$$

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Summary:

$$[L_x, L_y] = i\hbar L_z \quad [L_y, L_z] = i\hbar L_x \quad [L_z, L_x] = i\hbar L_y$$

Consider  $\mathbf{L}^2 = L_x^2 + L_y^2 + L_z^2$

$$\begin{aligned} [\mathbf{L}^2, L_z] &= [L_x^2 + L_y^2, L_z] \\ &= L_x[L_x, L_z] + [L_x, L_z]L_x + L_y[L_y, L_z] + [L_y, L_z]L_y \\ &= -i\hbar L_x L_y - i\hbar L_y L_x + i\hbar L_y L_x + i\hbar L_x L_y \\ &= 0 \end{aligned}$$

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Commutator relations for multiple particles

Consider N particles moving in one-dimension

$$\{X_1, X_2, \dots, X_N, P_1, P_2, \dots, P_N\}$$

$$[X_i, P_j] = i\hbar \delta_{ij}$$

$$[X_i, X_j] = 0$$

$$[P_i, P_j] = 0$$

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