Schmidt Orthogonalisation Technique

Starting from a set of linearly independent eigenfunctions $\{f_1, f_2, \ldots, f_n\}$ of a Hermitian operator with a degenerate eigenvalue, the application of the Schmidt Orthogonalization Technique gives a new set $\{F_1, F_2, \ldots, F_n\}$ of eigenfunctions with the same eigenvalue, such that the new set is an orthogonal set.

According to this procedure, the first new function F_1 is taken to be equal to f_1. F_2 is taken to be a linear combination of f_2 and F_1, i.e., to be $f_2 + c_{21}F_1$ (where c_{21} is a constant). Similarly, the other functions are defined. Thus we get:

$F_1 = f_1$, $\quad F_2 = f_2 + c_{21}F_1$, $\quad F_3 = f_3 + c_{32}F_2 + c_{31}F_1$

....

$F_j = f_j + {}_{i=1}\Sigma^{j-1}\, c_{ji}\, F_i$,

....

$F_n = f_n + {}_{i=1}\Sigma^{n-1}\, c_{ni}\, F_i$

Orthogonality of F_1 & F_2 gives $\langle F_1 | F_2\rangle = 0$, which means $\langle F_1 | f_2\rangle + c_{21}\langle F_1 | F_1\rangle = 0$, thus giving $c_{21} = -\langle F_1 | f_2\rangle / \langle F_1 | F_1\rangle$

Orthogonality of F_1 & F_3 gives $\langle F_1 | F_3\rangle = 0$, which means

$\langle F_1 | f_3\rangle + c_{32}\langle F_1 | F_2\rangle + c_{31}\langle F_1 | F_1\rangle = 0$, thus giving $c_{31} = -\langle F_1 | f_3\rangle / \langle F_1 | F_1\rangle$

(as $\langle F_1 | F_2\rangle = 0$ because of orthogonality of F_1 & F_2).

Similarly, $\langle F_2 | F_3\rangle = 0$ implies $c_{32} = -\langle F_2 | f_3\rangle / \langle F_2 | F_2\rangle$

Thus we arrive at a general formula for the coefficients c_{ji} (for $i < j$) as

$c_{ji} = \langle F_i | f_j\rangle / \langle F_i | F_i\rangle$. As the new functions F_j gets defined (as $F_j = f_j + {}_{i=1}\Sigma^{j-1}\, c_{ji}\, F_i$) when these coefficients are defined, the new orthogonal set of functions has been fully obtained.

Schwartz Inequality and Uncertainty Principle

For any two arbitrary well-behaved functions f and g the following relation is obeyed:

$4\langle f | f\rangle\langle g | g\rangle \geq (\langle f | g\rangle + \langle g | f\rangle)^2$ This relation is known as the **Schwartz inequality**.

Proof: Let $I = \langle (f + sg) | (f + sg)\rangle$ where s is an arbitrary real parameter. In the integral I, the integrand $|(f + sg)|^2$ is everywhere non-negative (i.e., positive or zero), and so I is positive, unless it happens that $f = -sg$ (in which case I is zero as the integrand becomes everywhere zero). So we have two possible cases: (1) $f = -sg$ in which case $I = 0$ and (2) $f \neq -sg$ in which case $I > 0$. However, by expanding the expression for I, we get

$I = \langle f | f\rangle + s\langle f | g\rangle + s^*\langle g | f\rangle + ss^*\langle g | g\rangle = \langle f | f\rangle + s(\langle f | g\rangle + \langle g | f\rangle) + s^2\langle g | g\rangle$

(as s is by definition real). Calling $\langle g | g\rangle = a$, $(\langle f | g\rangle + \langle g | f\rangle) = b$ and $\langle f | f\rangle = c$, we get $I = as^2 + bs + c$ with a, b, c being some constant integrals. Now considering the more general case (2) of $f \neq -sg$ and $I > 0$, we get $as^2 + bs + c > 0$ where s is real. This means that no real root for s exists for the equation $as^2 + bs + c = 0$, meaning that $(b^2 - 4ac)$ is negative giving only non-real complex roots for this quadratic equation. So we get, for $f \neq -sg$, $b^2 - 4ac < 0$ i.e., $4ac > b^2$

i.e., $4\langle f | f\rangle\langle g | g\rangle > (\langle f | g\rangle + \langle g | f\rangle)^2$ --------------- (i)

For the more specific case (1) of $f = -sg$, $\langle f | f\rangle = \langle (-sg) | (-sg)\rangle = s^2\langle g | g\rangle$ whereas $\langle f | g\rangle = -s^*\langle g | g\rangle = -s\langle g | g\rangle$ and $\langle g | f\rangle = -s\langle g | g\rangle$. These relations give:

$4\langle f \mid f\rangle\langle g \mid g\rangle = (\langle f \mid g\rangle + \langle g \mid f\rangle)^2$ --------------- (ii)
Thus, combining the two possible cases, we arrive at the Schwartz inequality:
$4\langle f \mid f\rangle \langle g \mid g\rangle \geq (\langle f \mid g\rangle + \langle g \mid f\rangle)^2$

In the **quantitative formulation of the (generalised) uncertainty principle** stated as **$\Delta A.\ \Delta G \geq \frac{1}{2} |\langle\psi \mid [\hat{A}, \hat{G}] \mid \psi\rangle|$**, the stated uncertainties ΔA and ΔG are nothing but the standard deviations in measurement of the physical observables A & G, where $\hat{A}$ & $\hat{G}$ are the corresponding Hermitian operators. This relation can be derived starting from the Schwartz inequality as follows:
From postulates of quantum mechanics, it is obvious that the standard deviations ΔA is given by: $\Delta A = (\langle\psi \mid \hat{A}^2 \mid \psi\rangle - \langle\psi \mid \hat{A} \mid \psi\rangle^2)^{1/2}$ (square root of the difference between average of square and square of average). In the Schwartz inequality, let us choose the arbitrary functions f & g as $f = (\hat{A} - \langle\hat{A}\rangle)\Psi$ and $g = i\,(\hat{G} - \langle\hat{G}\rangle)\Psi$, where $i = \sqrt{(-1)}$ and Ψ is the normalized system wavefunction (with $\langle\Psi \mid \Psi\rangle = 1$). Now

$\langle f \mid f\rangle = \langle(\hat{A} - \langle\hat{A}\rangle)\Psi \mid (\hat{A} - \langle\hat{A}\rangle)\Psi\rangle$
$= \langle\hat{A}\Psi \mid \hat{A}\Psi\rangle - \langle\hat{A}\Psi \mid \langle\hat{A}\rangle\Psi\rangle - \langle \langle\hat{A}\rangle\Psi \mid \hat{A}\Psi\rangle + \langle \langle\hat{A}\rangle\Psi \mid \langle\hat{A}\rangle\Psi\rangle$
$= \langle\Psi \mid \hat{A}^2\Psi\rangle - \langle\hat{A}\rangle \langle\Psi \mid \hat{A}\Psi\rangle - \langle\hat{A}\rangle^* \langle \Psi \mid \hat{A}\Psi\rangle + \langle\hat{A}\rangle \langle\hat{A}\rangle^* \langle \Psi \mid \Psi\rangle$ (as $\hat{A}$ is Hermitian)
$= \langle\Psi \mid \hat{A}^2 \mid \Psi\rangle - \langle\hat{A}\rangle \langle\Psi \mid \hat{A}\Psi\rangle - \langle\hat{A}\rangle \langle \Psi \mid \hat{A}\Psi\rangle + \langle\hat{A}\rangle \langle\hat{A}\rangle$ (as $\langle\hat{A}\rangle^* = \langle\hat{A}\rangle$)
$= \langle\Psi \mid \hat{A}^2 \mid \Psi\rangle - \langle\Psi \mid \hat{A} \mid \Psi\rangle^2 = (\Delta A)^2$
while $\langle g \mid g\rangle = \langle i(\hat{G} - \langle\hat{G}\rangle)\Psi \mid i(\hat{G} - \langle\hat{G}\rangle)\Psi\rangle$
$= i(-i) \langle(\hat{G} - \langle\hat{G}\rangle)\Psi \mid (\hat{G} - \langle\hat{G}\rangle)\Psi\rangle$
$= \langle(\hat{G} - \langle\hat{G}\rangle)\Psi \mid (\hat{G} - \langle\hat{G}\rangle)\Psi\rangle$
$= (\Delta G)^2$ (similarly)
Combining, it gives $\langle f \mid f\rangle \langle g \mid g\rangle = (\Delta A)^2 (\Delta G)^2$. Now let us look for $\langle f \mid g\rangle$ and $\langle g \mid f\rangle$:
$\langle f \mid g\rangle = \langle(\hat{A} - \langle\hat{A}\rangle)\Psi \mid i(\hat{G} - \langle\hat{G}\rangle)\Psi\rangle$
$= i \langle\hat{A}\Psi \mid \hat{G}\Psi\rangle - i \langle\hat{G}\rangle \langle\hat{A}\Psi \mid \Psi\rangle - i \langle\hat{A}\rangle^* \langle \Psi \mid \hat{G}\Psi\rangle + i \langle\hat{A}\rangle^* \langle\hat{G}\rangle \langle \Psi \mid \Psi\rangle$
$= i \langle\Psi \mid \hat{A}\hat{G} \mid \Psi\rangle - i \langle\hat{G}\rangle \langle\Psi \mid \hat{A} \mid \Psi\rangle - i \langle\hat{A}\rangle^* \langle \Psi \mid \hat{G} \mid \Psi\rangle + i \langle\hat{A}\rangle^* \langle\hat{G}\rangle \langle \Psi \mid \Psi\rangle$ (as $\hat{A}$, $\hat{G}$ Hermitian)
$= i \langle\Psi \mid \hat{A}\hat{G} \mid \Psi\rangle - i \langle\hat{A}\rangle\langle\hat{G}\rangle$ (as $\langle\hat{A}\rangle$, $\langle\hat{G}\rangle$ are real)
while $\langle g \mid f\rangle = -i \langle(\hat{G} - \langle\hat{G}\rangle)\Psi \mid (\hat{A} - \langle\hat{A}\rangle)\Psi\rangle = (-1)(i \langle\Psi \mid \hat{G}\hat{A} \mid \Psi\rangle - i \langle\hat{G}\rangle \langle\hat{A}\rangle)$ (similarly)
So, adding them we get, $\langle f \mid g\rangle + \langle g \mid f\rangle = i \langle\Psi \mid \hat{A}\hat{G} \mid \Psi\rangle - i \langle\Psi \mid \hat{G}\hat{A} \mid \Psi\rangle$
$= i \langle\Psi \mid (\hat{A}\hat{G} - \hat{G}\hat{A}) \mid \Psi\rangle = i \langle\Psi \mid [\, \hat{A}, \hat{G}\,] \mid \Psi\rangle$
Now application of the Schwartz inequality $4 \langle f \mid f\rangle\langle g \mid g\rangle \geq (\langle f \mid g\rangle + \langle g \mid f\rangle)^2$ gives
$4\, (\Delta A)^2 (\Delta G)^2 \geq (i \langle\Psi \mid [\, \hat{A}, \hat{G}\,] \mid \Psi\rangle)^2$ i.e., $4\, (\Delta A)^2 (\Delta G)^2 \geq - \langle\Psi \mid [\, \hat{A}, \hat{G}\,] \mid \Psi\rangle^2$
Taking modulus of square root on both sides we get
$2\, (\Delta A)\, (\Delta G) \geq |i \langle\Psi \mid [\, \hat{A}, \hat{G}\,] \mid \Psi\rangle|$ or, $2\, (\Delta A)\, (\Delta G) \geq |\langle\Psi \mid [\, \hat{A}, \hat{G}\,] \mid \Psi\rangle|$ i.e.,
$\Delta A\, \Delta G \geq \frac{1}{2} |\langle\Psi \mid [\, \hat{A}, \hat{G}\,] \mid \Psi\rangle|$, which is the (generalised) uncertainty principle.

For example, putting x in place of A and p_x in place of G, we get
$\Delta x\, \Delta p_x \geq \frac{1}{2} |\langle\Psi \mid [\, \hat{x}, \hat{p}_x\,] \mid \Psi\rangle|$. Now we know that
$[\, \hat{x}, \hat{p}_x\,]\, \Psi = x.(- i\hbar\, \partial/\partial x)\Psi - (- i\hbar\, \partial/\partial x)\, (x\Psi) = - i\hbar\, x\, \partial\Psi/\partial x + i\hbar\, \partial/\partial x\, (x\Psi)$
$= - i\hbar\, x\, \partial\Psi/\partial x + i\hbar\Psi + i\hbar\, x\, \partial\Psi/\partial x = i\hbar\, \Psi$, so that
$\langle\Psi \mid [\, \hat{x}, \hat{p}_x\,] \mid \Psi\rangle = \langle\Psi \mid i\hbar\, \Psi\rangle = i\hbar \langle\Psi|\Psi\rangle = i\hbar$ (as Ψ is normalised).

This gives $|\langle\Psi \mid [\ \hat{}x, \hat{}p_x\ ] \mid \Psi\rangle| = |\ i\ \hbar\ | = \hbar$, so that $\Delta x\ \Delta p_x \geq \frac{1}{2}\hbar = h/(4\pi)$, the well-known relation. Note: the RHS of the last inequality is $h/(4\pi)$ i.e., 5.273×10^{-35} J s, not $h/(2\pi)$.

The above concept is formulated also in the form of *compatible observables and incompatible observables*. A pair of mutually compatible observables are such a pair of observables (e.g., x & p_y) which can be simultaneously observed precisely, without any obstacle regarding the product of their uncertainties. For such a pair of observables, the commutator (e.g., [^x, ^p_y]) of their corresponding quantum-mechanical operators is zero. The compatibility theorem states just this: "For a pair of mutually compatible observables, the commutator of their corresponding quantum-mechanical operators is zero". On the other hand, incompatible observables are such a pair of observables (e.g., x & p_x) which *can't* be simultaneously observed precisely, with the product of their uncertainties (i.e., of standard deviations) can't be possible to become smaller than a certain minimum limit (this limit being the half of the modulus of the expectation value of the commutator of their corresponding quantum-mechanical operators, as per the generalised uncertainty principle mentioned above). For them the commutator of their corresponding quantum-mechanical operators is not zero.