

Parametric differentiation in quantum mechanics

Start with

$$\int_0^\pi \sin(ax) \sin(bx) dx = \frac{1}{2} \left[\frac{\sin(a-b)\pi}{a-b} - \frac{\sin(a+b)\pi}{a+b} \right] \quad a \neq \pm b. \quad (1)$$

Looking on the left side:

$$\frac{\partial^2}{\partial a^2} \left[\int_0^\pi (\sin ax)(\sin bx) dx \right] = \int_0^\pi \left(\frac{\partial^2}{\partial a^2} \sin ax \right) (\sin bx) dx = - \int_0^\pi (\sin ax)x^2(\sin bx) dx.$$

Looking on the right side:

$$\begin{aligned} \frac{\partial}{\partial u} \left[\frac{\sin u\pi}{u} \right] &= \frac{u\pi \cos u\pi - \sin u\pi}{u^2} \\ \frac{\partial^2}{\partial u^2} \left[\frac{\sin u\pi}{u} \right] &= \frac{u^2[\pi \cos u\pi - u\pi^2 \sin u\pi - \pi \cos u\pi] - 2u[u\pi \cos u\pi - \sin u\pi]}{u^4} \\ &= -\frac{\pi^2 \sin u\pi}{u} - \frac{2\pi \cos u\pi}{u^2} + \frac{2 \sin u\pi}{u^3}. \end{aligned}$$

Thus, the second derivative of equation (1) with respect to a becomes

$$\begin{aligned} \int_0^\pi (\sin ax)x^2(\sin bx) dx &= -\frac{1}{2} \frac{\partial^2}{\partial a^2} \left[\frac{\sin(a-b)\pi}{a-b} - \frac{\sin(a+b)\pi}{a+b} \right] \\ &= +\frac{1}{2} \left[\frac{\pi^2 \sin(a-b)\pi}{a-b} + \frac{2\pi \cos(a-b)\pi}{(a-b)^2} - \frac{2 \sin(a-b)\pi}{(a-b)^3} \right] \\ &\quad -\frac{1}{2} \left[\frac{\pi^2 \sin(a+b)\pi}{a+b} + \frac{2\pi \cos(a+b)\pi}{(a+b)^2} - \frac{2 \sin(a+b)\pi}{(a+b)^3} \right]. \end{aligned}$$

Recall that for N an integer, $\sin(N\pi) = 0$ and $\cos(N\pi) = (-1)^N$. This tells us that for n and m integers, (with $n \neq m$)

$$\langle n|x^2|m \rangle = \frac{2}{\pi} \int_0^\pi (\sin nx)x^2(\sin mx) dx = 2 \left[\frac{(-1)^{n-m}}{(n-m)^2} - \frac{(-1)^{n+m}}{(n+m)^2} \right].$$