Kronecker Product

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So why does the Kronecker product enter into quantum mechanics? It has to do with solutions to Schrodinger's equation when the potential is separable. Consider the general case of a two spin zero particles.

$$-\frac{\hbar^2}{2m}\nabla^2\psi(x,x') + V(x,x')\psi(x,x') = i\hbar\frac{\partial}{\partial t}\psi(x,x')$$

Now assume that the potential is separable i.e. $V(x,x') = V_a(x) + V_b(x')$. Then we can show that the solution can be written as $\psi(x,x') = \psi_a(x)\psi_b(x')$.

$$-\frac{\hbar^2}{2m}\nabla^2(\psi_a(x)\psi_b(x')) + (V_a(x) + V_b(x'))\psi_a(x)\psi_b(x') = i\hbar\frac{\partial}{\partial t}\psi_a(x)\psi_b(x')$$

$$-\frac{\hbar^2}{2m}[(\nabla^2\psi_a)\psi_b + \psi_a(\nabla^2\psi_b)] + (V_a + V_b)\psi_a\psi_b = i\hbar[(\partial_t\psi_a)\psi_b + \psi_a(\partial_t\psi_b)]$$

Now we divide by $\psi_a(x)\psi_b(x')$,

$$-\frac{\hbar^2}{2m}[(\nabla^2\psi_a)/\psi_a + (\nabla^2\psi_b)/\psi_b] + (V_a + V_b) = i\hbar[(\partial_t\psi_a)/\psi_a + (\partial_t\psi_b)/\psi_b]$$

Now rearranging,

$$-\frac{\hbar^2}{2m}(\nabla^2\psi_a)/\psi_a + V_a - i\hbar(\partial_t\psi_a)/\psi_a = \frac{\hbar^2}{2m}(\nabla^2\psi_b)/\psi_b - V_b + i\hbar(\partial_t\psi_b)/\psi_b]$$

Now the left and right hand sides are functions of mutually independent variables, so they must both be equal to the same constant, which can be set to zero without loss of generality by sifting the zero of potential. Therefore, we see that Schrodinger's equation holds for both particles separately, which is what we expect.

Really this logic is backwards. It makes more sense to start with two non-interacting particles, so two separate copies of Schrodinger's equation, and then proceed upwards to the conclusion that the product of the wave functions is again a solution to Schrodinger's equation, with the additional fact that the potential is separable. However the algebra is better motivated in the order that it is shown here.

Now we can see that this is the base case for the Kronecker product,

$$\psi_a \otimes \psi_b = \psi_a\psi_b$$

when the solutions are thought of as one component spinors. To see the pattern, we should check to see what happens when we use two-component spinors

$$\chi_a = \begin{pmatrix} \psi_{a1} \\ \psi_{a2} \end{pmatrix} \quad \text{and} \quad \chi_b = \begin{pmatrix} \psi_{b1} \\ \psi_{b2} \end{pmatrix}$$

It may not be obvious what it means for an operator to act on a vector. Say we take the derivative of a vector valued function. The derivative moves inside the vector to act on the functions,

$$\partial_x\mathbf{V}(x) = \partial_x\begin{pmatrix} f(x) \\ g(x) \end{pmatrix} = \begin{pmatrix} \partial_x f(x) \\ \partial_x g(x) \end{pmatrix}$$

This is not an assumption, it is forced by the definition of the derivative. Therefore the Hamiltonian operator can be moved inside or outside a vector. The reason this can be confusing is that there are some operators that are specifically designed to act on the vectors themselves (such as spin operators in the form of Pauli matrices), and thus cannot be moved inside to act on the vector's components.

Before continuing we need to prove a lemma about how the Hamiltonian acts on products of wave functions. If $\hat{H}_a$ is a linear operator constructed from $\hat{x}$ and $\hat{p}$, and if $\hat{H}_b$ is a linear operator constructed from $\hat{x}'$ and $\hat{p}'$, and $\hat{H} = \hat{H}_a + \hat{H}_b$, then

$$\hat{H}(\psi_a(x)\psi_b(x')) = (\hat{H}_a\psi_a(x))\psi_b(x') + \psi_a(x)(\hat{H}_b\psi_b(x'))$$

The proof is based on the product rule and the fact that the primed and unprimed operators are independent.

$$\hat{H}(\psi_a(x)\psi_b(x')) = \hat{H}_a(\psi_a(x)\psi_b(x')) + \hat{H}_b(\psi_a(x)\psi_b(x'))$$
$$= (\hat{H}_a\psi_a(x))\psi_b(x') + \psi_a(x)(\hat{H}_a\psi_b(x')) + (\hat{H}_b\psi_a(x))\psi_b(x') + \psi_a(x)(\hat{H}_b\psi_b(x'))$$

The middle two terms drop out because of independence of variables and we are left with the statement we wished to show. Question: How can we prove that $\hat{x}\psi(x') = 0$?

Now one of the fundamental properties of the Schrodinger equation is that it is linear. That is what allows us to express states as linear combinations of energy eigenstates for example. Spinors are solutions to Schrodinger's equation, so spinors must have this property also. Question: How can we rigorously prove that it has to be bilinear? i.e. $(A+B)*C = A*C + B*C$ and $A*(B+C) = A*B + A*C$.

So we want to find a bilinear operation $*$ that combines all the information from two states and forms a new state. Then we will show that $*$ has to be the Kronecker product $\otimes$.

Since $*$ is bilinear,

$$\partial_x(\chi_a(x) * \chi_b(x')) = \lim_{h\to 0}(\chi_a(x+h) * \chi_b(x') - \chi_a(x) * \chi_b(x'))/h$$
$$= \lim_{h\to 0}(\chi_a(x+h) - \chi_a(x))/h * \chi_b(x') = (\partial_x\chi_a(x)) * \chi_b(x')$$

Therefore, a bilinear operation $*$ must satisfy

$$\hat{H}(\chi_a * \chi_b) = (\hat{H}_a\chi_a) * \chi_b + \chi_a * (\hat{H}_b\chi_b)$$

If we assume that $*$ is $\otimes$ and expand the definition of the Kronecker product,

$$\begin{pmatrix} \hat{H}(\psi_{a1}\psi_{b1}) \\ \hat{H}(\psi_{a1}\psi_{b2}) \\ \hat{H}(\psi_{a2}\psi_{b1}) \\ \hat{H}(\psi_{a2}\psi_{b2}) \end{pmatrix} = \begin{pmatrix} \hat{H}_a(\psi_{a1})\psi_{b1} \\ \hat{H}_a(\psi_{a1})\psi_{b2} \\ \hat{H}_a(\psi_{a2})\psi_{b1} \\ \hat{H}_a(\psi_{a2})\psi_{b2} \end{pmatrix} + \begin{pmatrix} \psi_{a1}\hat{H}_b(\psi_{b1}) \\ \psi_{a1}\hat{H}_b(\psi_{b2}) \\ \psi_{a2}\hat{H}_b(\psi_{b1}) \\ \psi_{a2}\hat{H}_b(\psi_{b2}) \end{pmatrix}$$

And this equation we recognize to be true by the lemma, so we have shown that $\otimes$ works as the needed operator $*$. If you try defining $*$ by

$$\chi_a * \chi_b = \begin{pmatrix} \psi_{a1} \\ \psi_{a2} \\ \psi_{b1} \\ \psi_{b2} \end{pmatrix}$$

you will find that it does not satisfy bilinearity. If you define $*$ by

$$\chi_a * \chi_b = \begin{pmatrix} \psi_{a1}\psi_{b1} \\ \psi_{a2}\psi_{b2} \end{pmatrix}$$

it will be bilinear, but you will have lost information since you started with four independent functions and now have only two. I believe it turns out that the Kronecker product is the only definition of $*$ that works without redundancies.