Linear Algebra and Quantum Mechanics

1. Dirac Notation: Bra's and Ket's

Eventually we all get tired of writing integrals. Working in the early 1930's, a man named Paul Dirac got tired of writing integrals and decided to replace integrals like

$$\overset{\text{integral over all space}}{\int} d\boldsymbol{\tau} \left(\Psi_1^*(\boldsymbol{\tau}) \overset{\xleftarrow{\text{can operate backwards}}}{\underbrace{\hat{C}(\boldsymbol{\tau})}_{\xrightarrow{\text{can operate forwards}}}} \Psi_2 \underset{\text{just a "dummy" variable}}{(\boldsymbol{\tau})} \right) \tag{1}$$

with a compact notation,

$$\left\langle \Psi_1 \middle| \hat{C} \middle| \Psi_2 \right\rangle \tag{2}$$

- There is no mention of the limits of integration because this is always "clear from the problem" and, in any event, can always be taken to be all of real space.
- Because of the Hermitian property of the operator, $\hat{C}(\boldsymbol{\tau})$ it can operate either "forwards" (on $\Psi_2(\boldsymbol{\tau})$) or "backwards" (on $\Psi_1^*(\boldsymbol{\tau})$).
- The variable of integration does not need to be specified since it is just a "dummy variable." I.e., you can change $\boldsymbol{\tau}$ to another variable with the same dimensionality, $\mathbf{u}$, without changing the interpretation of Eq. (1).

Dirac called the first part of the notation, with the complex-conjugated wavefunction, a "bra", and the second part a ket.

$$\underset{\text{bra}}{\langle \Psi_1 |} \hat{C} \underset{\text{ket}}{| \Psi_2 \rangle} \tag{3}$$

Together you have a "bra $\hat{C}$ ket". Who says physicists are immune to bad puns?

Everything before the first vertical line in a bracket is automatically complex conjugated. Sometimes the second vertical line is omitted, and then one has notation like

$$\left\langle \Psi_1 \middle| \hat{C}\Psi_2 \right\rangle = \left\langle \hat{C}\Psi_1 \middle| \Psi_2 \right\rangle \tag{4}$$

This is a very compact notation. It was basically motivated by the tendency of physicists and mathematicians to write expectation values (that is, mean values) as $\langle C \rangle$. From there it is a short notational step to:

$$\langle C \rangle = \left\langle \Psi \middle| \hat{C} \middle| \Psi \right\rangle \tag{5}$$

When you see an bra all by itself, it indicates the complex conjugate of the wavefunction:

$$\langle \Psi | = \Psi^*(\boldsymbol{\tau}). \tag{6}$$

An isolated ket means

$$| \Psi \rangle = \Psi(\boldsymbol{\tau}). \tag{7}$$

Dirac has Asperger's syndrome and was quite immune, it seems, from making sexually suggestive remarks about "bra"s. It seems to have never occurred to him. However, there are strange mathematical objects, which I saw in a physics seminar a long time ago, called "padded bras."

2. Linear Algebra and the Analogy to Quantum Mechanics

Aside from its utility for making jokes (which are in short supply in physics seminars) and the fact it saves one from writer's cramp, physicists like Dirac notation because it makes it easier to see the analogies between linear algebra and the mathematics of quantum mechanics. Almost every result in linear algebra has an analogue in quantum mechanics.

Quantum Mechanics	Linear Algebra
Infinite-dimensional complex-valued vector space. ("Hilbert space.")	Finite-dimensional complex-valued vector space. (Could also be a real-valued vector space.)
Wavefunctions, $\Psi(\boldsymbol{\tau}) = \lvert\Psi\rangle$.	*d*-dimensional vectors, $\mathbf{v}$
Complex-conjugate wavefunctions, $\Psi^*(\boldsymbol{\tau}) = \langle\Psi\rvert$	Hermitian transpose of vectors, $\mathbf{v}^\dagger = (\mathbf{v}^*)^T = (\mathbf{v}^T)^*$.
Space of all wavefunctions is the space of all $\Psi(\boldsymbol{\tau})$ for which $$\infty > \int \Psi^*(\boldsymbol{\tau})\Psi(\boldsymbol{\tau})\,d\boldsymbol{\tau} = \langle\Psi\vert\Psi\rangle$$	Space of all vectors is the space of all $\mathbf{v}$ for which $$\infty > \mathbf{v}^\dagger\mathbf{v}$$
Norm of wavefunctions is $$\lVert\Psi\rVert = \sqrt{\int \Psi^*(\boldsymbol{\tau})\Psi(\boldsymbol{\tau})\,d\boldsymbol{\tau}} = \sqrt{\langle\Psi\vert\Psi\rangle}$$	Norm of vectors is $$\lVert\mathbf{v}\rVert = \sqrt{\mathbf{v}^\dagger\mathbf{v}}$$
Inner product between wavefunctions is $$\int \Psi_1^*(\boldsymbol{\tau})\Psi_2(\boldsymbol{\tau})\,d\boldsymbol{\tau} = \langle\Psi_1\vert\Psi_2\rangle$$	Inner product ("dot" product) between vectors is $\mathbf{v}_1^\dagger\mathbf{v}_2 = \mathbf{v}_1^*\cdot\mathbf{v}_2$
Linear Hermitian Operators, $$\int \Psi_1^*(\boldsymbol{\tau})\hat{C}(\boldsymbol{\tau})\Psi_2(\boldsymbol{\tau})\,d\boldsymbol{\tau} = \int\left(\hat{C}(\boldsymbol{\tau})\Psi_1(\boldsymbol{\tau})\right)^*\Psi_2(\boldsymbol{\tau})\,d\boldsymbol{\tau} = \int \hat{C}^*(\boldsymbol{\tau})\Psi_1^*(\boldsymbol{\tau})\Psi_2(\boldsymbol{\tau})\,d\boldsymbol{\tau}$$ $$\left\langle\Psi_1\middle\vert\hat{C}\middle\vert\Psi_2\right\rangle = \left\langle\Psi_1\middle\vert\hat{C}\Psi_2\right\rangle = \left\langle\hat{C}\Psi_1\middle\vert\Psi_2\right\rangle$$	Hermitian Matrices, $\mathbf{C} = (\mathbf{C}^*)^T = \mathbf{C}^\dagger$. $$\mathbf{v}_1^\dagger\mathbf{C}\mathbf{v}_2 = (\mathbf{C}\mathbf{v}_1)^\dagger\,\mathbf{v}_2$$

<table>
<tr>
<td>Eigenvalues of Linear, Hermitian, operators are real and the corresponding eigenvectors can be chosen to form a complete, orthonormal, set

$$\hat{C}(\boldsymbol{\tau})\Psi_k(\boldsymbol{\tau}) = c_k\Psi_k(\boldsymbol{\tau}) \qquad c_k \in \mathbb{R}$$

$$\int \Psi_k^*(\boldsymbol{\tau})\Psi_l(\boldsymbol{\tau})\,d\boldsymbol{\tau} = \delta_{kl}$$

$$\hat{C}\left|\Psi_k\right\rangle = c_k\left|\Psi_k\right\rangle$$

$$\left\langle\Psi_k\middle|\Psi_l\right\rangle = \delta_{kl}$$

Any wavefunction can be written as:

$$\Phi(\boldsymbol{\tau}) = \sum_{k=0}^{\infty} b_k\Psi_k(\boldsymbol{\tau}) \qquad b_k = \int \Psi_k^*(\boldsymbol{\tau})\Phi(\boldsymbol{\tau})\,d\boldsymbol{\tau}$$

$$\left|\Phi\right\rangle = \sum_{k=0}^{\infty} b_k\left|\Psi_k\right\rangle \qquad b_k = \left\langle\Psi_k\middle|\Phi\right\rangle$$
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<td>Eigenvalues of Hermitian matrices are real and the corresponding eigenvectors can be chosen to form a complete, orthonormal, set

$$\mathbf{C}\mathbf{v}_k = c_k\mathbf{v}_k \qquad c_k \in \mathbb{R}$$

$$\mathbf{v}_k^\dagger\mathbf{v}_l = \delta_{kl}$$

Any vector can be written as

$$\mathbf{u} = \sum_{k=0}^{d-1} b_k\mathbf{v}_k \qquad b_k = \mathbf{v}_k^\dagger\mathbf{u}$$
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<td>Inner product expressed with a basis set.

$$\Phi(\boldsymbol{\tau}) = \sum_{k=0}^{\infty} b_k\Psi_k(\boldsymbol{\tau}) = \sum_{k=0}^{\infty} b_k\left|\Psi_k\right\rangle$$

$$\varphi(\boldsymbol{\tau}) = \sum_{k=0}^{\infty} a_k\Psi_k(\boldsymbol{\tau}) = \sum_{k=0}^{\infty} a_k\left|\Psi_k\right\rangle$$

$$\int \Phi^*(\boldsymbol{\tau})\varphi(\boldsymbol{\tau})\,d\boldsymbol{\tau} = \left\langle\Phi\middle|\varphi\right\rangle = \sum_{k=0}^{\infty} b_k^* a_k$$

Suggested Exercise: Derive this result.
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<td>Inner product expressed with a basis set

$$\mathbf{u} = \sum_{k=0}^{d-1} b_k\mathbf{v}_k$$

$$\mathbf{w} = \sum_{k=0}^{d-1} a_k\mathbf{v}_k$$

$$\mathbf{u}^\dagger\mathbf{w} = \sum_{k=0}^{d-1} b_k^* a_k$$
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Linear, Hermitian, operator expressed with a basis set

$$\hat{C} \Leftrightarrow \sum_{k=0}^{\infty}\sum_{l=0}^{\infty}\Psi_k(\boldsymbol{\tau})\left(\int \Psi_k^*(\boldsymbol{\tau}'')\hat{C}(\boldsymbol{\tau}'')\Psi_l(\boldsymbol{\tau}'')d\boldsymbol{\tau}''\right)\Psi_l^*(\boldsymbol{\tau}')$$

$$= \sum_{k=0}^{\infty}\sum_{l=0}^{\infty}\Psi_k(\boldsymbol{\tau})c_{kl}\Psi_l^*(\boldsymbol{\tau}')$$

$$\hat{C} \Leftrightarrow \sum_{k=0}^{\infty}\sum_{l=0}^{\infty}|\Psi_k\rangle\left\langle\Psi_k\middle|\hat{C}\middle|\Psi_l\right\rangle\langle\Psi_l| = \sum_{k=0}^{\infty}\sum_{l=0}^{\infty}|\Psi_k\rangle c_{kl}\langle\Psi_l|$$

$$c_{kl} = c_{lk}^* = \int \Psi_k^*(\boldsymbol{\tau}'')\hat{C}(\boldsymbol{\tau}'')\Psi_l(\boldsymbol{\tau}'')d\boldsymbol{\tau}'' = \left\langle\Psi_k\middle|\hat{C}\middle|\Psi_l\right\rangle$$
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Matrix expressed with a basis set

$$\mathbf{C} = \sum_{k=0}^{d-1}\sum_{l=0}^{d-1}\mathbf{v}_k\left(\mathbf{v}_k^\dagger\mathbf{C}\mathbf{v}_l\right)\mathbf{v}_l^\dagger = \sum_{k=0}^{d-1}\sum_{l=0}^{d-1}\mathbf{v}_k c_{kl}\mathbf{v}_l^\dagger$$

$$c_{kl} = \mathbf{v}_k^\dagger\mathbf{C}\mathbf{v}_l$$
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Action of a linear, Hermitian, operator on a wavefunction,

$$\Phi(\boldsymbol{\tau}) = \sum_{k=0}^{\infty}b_k\Psi_k(\boldsymbol{\tau}) = \sum_{k=0}^{\infty}b_k|\Psi_k\rangle$$

$$b_k = \int\Psi_k^*(\boldsymbol{\tau})\Phi(\boldsymbol{\tau})d\boldsymbol{\tau} = \langle\Psi_k|\Phi\rangle$$

$$c_{kl} = c_{lk}^* = \int \Psi_k^*(\boldsymbol{\tau}'')\hat{C}(\boldsymbol{\tau}'')\Psi_l(\boldsymbol{\tau}'')d\boldsymbol{\tau}'' = \left\langle\Psi_k\middle|\hat{C}\middle|\Psi_l\right\rangle$$

$$\hat{C}(\boldsymbol{\tau})\Phi(\boldsymbol{\tau}) = \sum_{k=0}^{\infty}\sum_{l=0}^{\infty}\int\Psi_k(\boldsymbol{\tau})\left(\int \Psi_k^*(\boldsymbol{\tau}'')\hat{C}(\boldsymbol{\tau}'')\Psi_l(\boldsymbol{\tau}'')d\boldsymbol{\tau}''\right)\Psi_l^*(\boldsymbol{\tau}')\Phi(\boldsymbol{\tau}')d\boldsymbol{\tau}'$$

$$= \sum_{k=0}^{\infty}\Psi_k(\boldsymbol{\tau})\sum_{l=0}^{\infty}c_{kl}b_l$$

$$\hat{C}|\Phi\rangle = \sum_{k=0}^{\infty}\sum_{l=0}^{\infty}|\Psi_k\rangle\left\langle\Psi_k\middle|\hat{C}\middle|\Psi_l\right\rangle\langle\Psi_l|\Phi\rangle$$

$$= \sum_{k=0}^{\infty}|\Psi_k\rangle\sum_{l=0}^{\infty}c_{kl}b_l$$

Suggested Exercise: Derive this result.
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Action of a matrix on a vector,

$$\mathbf{u} = \sum_{k=0}^{d-1}b_k\mathbf{v}_k \qquad b_k = \mathbf{v}_k^\dagger\mathbf{u}$$

$$c_{kl} = \mathbf{v}_k^\dagger\mathbf{C}\mathbf{v}_l$$

$$\mathbf{C}\mathbf{u} = \sum_{k=0}^{d-1}\sum_{l=0}^{d-1}\mathbf{v}_k c_{kl}\mathbf{v}_l^\dagger\mathbf{u}$$

$$= \sum_{k=0}^{d-1}\mathbf{v}_k\sum_{l=0}^{d-1}c_{kl}b_l$$

This is equal to the usual formula if the basis is chosen so that $\mathbf{v}_k$ is the vector that is all zeros, except for a 1 in the k-1st position.
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Product of two linear, Hermitian, Operators

$$\hat{C} \Leftrightarrow \sum_{k=0}^{\infty}\sum_{l=0}^{\infty} \left|\Psi_k\right\rangle \left\langle \Psi_k \middle| \hat{C} \middle| \Psi_l \right\rangle \left\langle \Psi_l \right| = \sum_{k=0}^{\infty}\sum_{l=0}^{\infty} \left|\Psi_k\right\rangle c_{kl} \left\langle \Psi_l \right|$$

$$\hat{D} \Leftrightarrow \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} \left|\Psi_m\right\rangle \left\langle \Psi_m \middle| \hat{D} \middle| \Psi_n \right\rangle \left\langle \Psi_n \right| = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} \left|\Psi_m\right\rangle d_{mn} \left\langle \Psi_n \right|$$

$$\begin{aligned}\hat{C}\hat{D} &= \sum_{k=0}^{\infty}\sum_{l=0}^{\infty}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty} \left|\Psi_k\right\rangle \left\langle \Psi_k \middle| \hat{C} \middle| \Psi_l \right\rangle \left\langle \Psi_l \middle| \Psi_m \right\rangle \left\langle \Psi_m \middle| \hat{D} \middle| \Psi_n \right\rangle \left\langle \Psi_n \right| \\ &= \sum_{k=0}^{\infty}\sum_{l=0}^{\infty}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty} \left|\Psi_k\right\rangle c_{kl}\delta_{lm} d_{mn} \left\langle \Psi_n \right| \\ &= \sum_{k=0}^{\infty}\sum_{l=0}^{\infty}\sum_{n=0}^{\infty} \left|\Psi_k\right\rangle c_{kl} d_{ln} \left\langle \Psi_n \right| \\ &= \sum_{k=0}^{\infty} \left|\Psi_k\right\rangle \sum_{n=0}^{\infty} \left\langle \Psi_n \right| \sum_{l=0}^{\infty} c_{kl} d_{ln}\end{aligned}$$

Suggested Exercise: Derive the expression for $\left\langle \Phi \middle| \hat{C}\hat{D} \middle| \Phi \right\rangle$ in this basis set.

Product of two matrices:

$$\mathbf{C} = \sum_{k=0}^{d-1}\sum_{l=0}^{d-1} \mathbf{v}_k \left(\mathbf{v}_k^\dagger \mathbf{C} \mathbf{v}_l\right) \mathbf{v}_l^\dagger = \sum_{k=0}^{d-1}\sum_{l=0}^{d-1} \mathbf{v}_k c_{kl} \mathbf{v}_l^\dagger$$

$$\mathbf{D} = \sum_{m=0}^{d-1}\sum_{n=0}^{d-1} \mathbf{v}_m \left(\mathbf{v}_m^\dagger \mathbf{D} \mathbf{v}_n\right) \mathbf{v}_n^\dagger = \sum_{m=0}^{d-1}\sum_{n=0}^{d-1} \mathbf{v}_m d_{mn} \mathbf{v}_n^\dagger$$

$$\begin{aligned}\mathbf{CD} &= \sum_{k=0}^{d-1}\sum_{l=0}^{d-1}\sum_{m=0}^{d-1}\sum_{n=0}^{d-1} \mathbf{v}_k c_{kl} \mathbf{v}_l^\dagger \mathbf{v}_m d_{mn} \mathbf{v}_n^\dagger \\ &= \sum_{k=0}^{d-1}\sum_{l=0}^{d-1}\sum_{m=0}^{d-1}\sum_{n=0}^{d-1} \mathbf{v}_k c_{kl}\delta_{lm} d_{mn} \mathbf{v}_n^\dagger \\ &= \sum_{k=0}^{d-1}\sum_{l=0}^{d-1}\sum_{n=0}^{d-1} \mathbf{v}_k c_{kl} d_{ln} \mathbf{v}_n^\dagger \\ &= \sum_{k=0}^{d-1} \mathbf{v}_k \sum_{n=0}^{d-1} \mathbf{v}_n^\dagger \sum_{l=0}^{d-1} c_{kl} d_{ln}\end{aligned}$$

This is equal to the usual formula if the basis is chosen so that $\mathbf{v}_k$ is the vector that is all zeros, except for a 1 in the *k*-1st position.