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Tranformation Theory

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References

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The general structure of quantum mechanical calculations

There are three steps in every quantum mechanical calculation:

(1) Prepare a system

Let a state be prepared by measuring an observable $\hat{A}$. If

$$\hat{A}\psi_a = a\psi_a, \quad \{a, \psi_a\} \sim \text{the set of eigenvalues, eigenvectors of } \hat{A},$$

we can start the system in

$$\Psi(0) = \psi_a$$

by choosing systems for which an observation of $\hat{A}$ at $t = 0$ reveals a.

(2) Wait in time

If $\hat{H}\chi_n = E_n\chi_n$, the initial state

$$\Psi(0) = \sum_n \langle \chi_n | \psi_a \rangle \, \chi_n$$

evolves in time into

$$\Psi(t) = \sum_n e^{-iE_n t/\hbar} \langle \chi_n | \psi_a \rangle \, \chi_n .$$

(3) Observe $\hat{B}$

If $\hat{B}\phi_b = b\phi_b$, observation of $\hat{B}$ will reveal the value b with probability

$$\left| \sum_n \langle \phi_b | \chi_n \rangle \, e^{-iE_n t/\hbar} \langle \chi_n | \psi_a \rangle \right|^2 .$$

Unitary transformations

A transformation $\hat{U}$ is *linear* if

$$\hat{U}(a\psi_1 + b\psi_2) = a(\hat{U}\psi_1) + b(\hat{U}\psi_2)$$

for all a, b, ψ_1, ψ_2. $\hat{U}$ is *unitary* if

$$\left\langle \hat{U}\psi_1 | \hat{U}\psi_2 \right\rangle = \langle \psi_1, \psi_2 \rangle$$

for all ψ_1, ψ_2.

The 3D vector analogue for this would be that

$$(\hat{U}\vec{v}) \cdot (\hat{U}\vec{w}) = \vec{v} \cdot \vec{w}$$

for all $\vec{v}, \vec{w}$. This is valid for *rotations* in 3D. Thus a unitary transformation is a complex multidimensional extension of a rotation. [For *real* multidimensional vectors these are called *orthogonal* transformations.]

Matrix representations

In an orthonormal basis set $\{\phi_n\}$, $\hat{U}$ would have a matrix representation

$$U_{mn} = \langle \phi_m | \hat{U}\phi_n \rangle.$$

If ψ_a, ψ_b are two (arbitrary) vectors with the matrix representations

$$\psi_a = \sum_n a_n \phi_n,$$
$$\psi_b = \sum_n b_n \phi_n,$$

then

$$\langle \psi_a | \psi_b \rangle = \sum_n a_n^* b_n.$$

Since

$$\hat{U}\psi_a = \sum_n a_n \hat{U}\phi_n = \sum_{n,k} a_n \langle \phi_k | \hat{U}\phi_n \rangle \phi_k = \sum_{k,n} \phi_k U_{kn} a_n,$$

$$\langle \hat{U}\psi_a | \hat{U}\psi_b \rangle = \sum_{k,m,n} U_{km}^* a_m^* U_{kn} b_n$$

Thus $\hat{U}$ is unitary $\Longleftrightarrow$

$$\sum_n a_n^* b_n = \sum_{k,m,n} U_{km}^* a_m^* U_{kn} b_n, \qquad \text{all } a_m, b_n$$

$$a_n^* = \sum_{k,m} a_m^* U_{km}^* U_{kn}, \qquad \text{all } a_m$$

$$\delta_{mn} = \sum_k U_{km}^* U_{kn}. \tag{1}$$

Now the inverse operator $\hat{U}^{-1}$ is the operator for which

$$\hat{U}^{-1} \cdot \hat{U} = \hat{1},$$

with $\hat{1}$ the *identity* operator. Since the matrix representation for $\hat{1}$ is δ_{mn},

$$\begin{aligned}\delta_{mn} &= \langle \phi_m | \hat{U}^{-1} \hat{U} | \phi_n \rangle \\ &= \sum_k \left[\hat{U}^{-1} \right]_{mk} U_{kn}.\end{aligned}$$

Comparison with (1) shows that $\hat{U}$ is *unitary* $\Longleftrightarrow$ $\left[\hat{U}^{-1} \right]_{mn} = U_{nm}^*$.

Contrast these two cases: If you transpose and take the complex conjugate of a matrix, you get

(i) the original matrix if the operator is *Hermitian*,

(ii) the inverse operator if the operator is *unitary*.

Basis set transformations are unitary

Let $\{\phi_n\}$ be an orthonormal basis set, let $\hat{T}$ be a linear transformation, and let

$$\psi_k = \hat{T} \phi_k$$

be the vector into which $\hat{T}$ transforms ϕ_k. In matrix form,

$$\psi_k = \sum_n \langle \phi_n | \hat{T} \phi_k \rangle \, \phi_n = \sum_n T_{nk} \, \phi_n$$

with

$$T_{nk} = \langle \phi_n | \psi_k \rangle = \langle \phi_n | \hat{T} \phi_k \rangle.$$

$\hat{T}$ will give a transformation to a new orthonormal basis set if

$$\begin{aligned}\delta_{k\ell} &= \langle \psi_k | \psi_\ell \rangle \\ &= \sum_{m,n} \langle T_{mk}\phi_m | T_{n\ell}\phi_n \rangle \\ &= \sum_{m,n} T^*_{mk} T_{n\ell} \langle \phi_m | \phi_n \rangle \\ &= \sum_n T^*_{nk} T_{n\ell}\end{aligned}$$

which shows (compare this with (1)) that T_{ij} is the matrix representation of a unitary transformation. That is, a "rotation" of an orthonormal basis set gives a new orthonormal basis set.

Of course the T_{nk} are the components of ψ_k in the basis set $\{\phi_n\}$. Writing $T_{nk} = \psi_k^{(n)}$,

$$[T]_{nk} = \begin{bmatrix} \psi_1^{(1)} & \psi_2^{(1)} & \cdots \\ \psi_1^{(2)} & \psi_2^{(2)} & \cdots \\ \vdots & \vdots & \cdots \end{bmatrix} = \left[\vec{\psi}_1 \,|\, \vec{\psi}_2 \,|\, \cdots \right]$$

and the fact that $[T]_{nk} = [T^{-1}]^*_{kn}$ just reflects the orthonormality of the vectors $\{\psi_k\}$ and

$$[T^{-1}]_{kn} = [T^*]_{nk} = \langle \psi_n | \phi_k \rangle^* = \langle \phi_k | \psi_n \rangle$$

are just the matrix elements of the transformation from the $\{\psi_k\}$ basis set to the $\{\phi_n\}$ basis set.

Translations in space and time are unitary

If a system in state $\Psi(\boldsymbol{r})$ is translated a distance $\boldsymbol{d}$ in space, the state is converted into

$$\begin{aligned}\Psi(\boldsymbol{r}-\boldsymbol{d}) &= \sum_{n=0}^{\infty} \frac{1}{n!} \left(-\boldsymbol{d} \cdot \frac{\partial}{\partial \boldsymbol{r}} \right)^n \Psi(\boldsymbol{r}) = \sum_{n=0}^{\infty} \frac{1}{n!} \left(-\frac{i}{\hbar} \boldsymbol{d} \cdot \frac{\hbar}{i} \frac{\partial}{\partial \boldsymbol{r}} \right)^n \Psi(\boldsymbol{r}) \\ &= \sum_{n=0}^{\infty} \frac{1}{n!} \left(-\frac{i}{\hbar} \boldsymbol{d} \cdot \hat{\boldsymbol{p}} \right)^n \Psi(\boldsymbol{r}) = e^{-i\boldsymbol{d}\cdot\hat{\boldsymbol{p}}/\hbar}\, \Psi(\boldsymbol{r})\end{aligned}$$

That is, translations in space are generated by the opeartor

$$\hat{T}_{space} = e^{-i\boldsymbol{d}\cdot\hat{\boldsymbol{p}}/\hbar}$$

Since

$$\left\langle e^{-id\cdot\hat{p}/\hbar}\,\psi_1|e^{-id\cdot\hat{p}/\hbar}\,\psi_2\right\rangle = \left\langle \psi_1|e^{id\cdot\hat{p}/\hbar}\,e^{-id\cdot\hat{p}/\hbar}\,\psi_2\right\rangle = \langle\psi_1,\psi_2\rangle\,,$$

$\hat{T}_{space}$ is unitary. We say that p_x, the momentum conjugate to x, generates translation down the x-axis.

Time evolution changes

$$\Psi_0 \to \Psi(t) = e^{-i\hat{H}\,t/\hbar}\,\Psi_0$$

The operator $e^{-i\hat{H}\,t/\hbar}$ that generates time evolution has the same form as $\hat{T}_{space}$. Time evolution is just translation down the time axis.

In both these example, a *unitary* operator is associated with an *Hermitian* operator,

$$\text{‘unitary’} = e^{-i\,\times\,\text{constant}\,\times\,\text{‘Hermitian’}}$$

The quantum calculation revisited

Since $e^{-i\hat{H}t/\hbar}\chi_n = e^{-iE_nt/\hbar}\chi_n$, the probability of seeing 'b' after starting a system in ψ_a and waiting a time t can be written

$$\left|\sum_{m,n}\langle\phi_b|\chi_m\rangle\langle\chi_m|e^{-i\hat{H}t/\hbar}\chi_n\rangle\langle\chi_n|\psi_a\rangle\right|^2 .$$

Let $\quad R_{na} = \langle\chi_n|\psi_a\rangle$

generate the unitary transformation associated with the basis set transformation

$$\{\psi_a\} \to \{\chi_n\},$$

while $S_{bn} = \langle\phi_b|\chi_n\rangle$ generates the $\{\chi_n\} \to \{\phi_b\}$ transformation.

If

$$U_{mn}(t) = \langle\chi_m|e^{-i\hat{H}t/\hbar}\chi_n\rangle = e^{-E_nt/\hbar}\delta_{mn},$$

then

$$\sum_k U^*_{km}(t)U_{kn}(t) = \sum_k e^{iE_mt/\hbar}\delta_{km}e^{-iE_nt/\hbar}\delta_{kn} = \delta_{mn}.$$

Symbolically,

$$\Psi(t) = \hat{U}(t)\Psi(0), \qquad \text{with} \quad \hat{U}(t) = e^{-i\hat{H}t/\hbar}$$

$\hat{U}(t)$ is a unitary transformation.

Putting all this together, the sought probability is

$$\left|\sum_{m,n} S_{bm}U_{mn}(t)R_{na}\right|^2 = \left|[\hat{S}\hat{U}(t)\hat{R}]_{ba}\right|^2.$$

The calculational problem consists of making three unitary transformations. We start from a basis set fixed by $\hat{A}$, rotate to a basis set fixed by $\hat{H}$, rotate $e^{-i\hat{H}t/\hbar}$, and then transform to a basis set fixed by $\hat{B}$.

Dirac's abstraction

Suppose we prepare a system in state ψ_a at $t = 0$ and then immediately measure 'x'. According to the previous calculation, we see 'x' with probability $|\langle\phi_x|\psi_a\rangle|^2$. Dirac argued that, since there were many basis sets in which ψ_a could be represented, one should distinguish the idea of an abstract representation of a state from the idea of a particular representation in some basis set.

Suppose a system is prepared in a state ψ. To represent this abstractly we write

$$|\psi\rangle$$

for the state vector. Now the probability of seeing 'b' in this state is

$$|\langle\phi_b|\psi\rangle|^2.$$

But it is only the label 'b' in this expression which has some information content. If we replace $\phi_b \to |b\rangle$, then

$$\hat{B}|b\rangle = b|b\rangle$$

and the probability of seeing 'b' is

$$|\langle b|\psi\rangle|^2.$$

From this point of view the wave function of Schrödinger is just

$$\psi(x) = \langle x|\psi\rangle.$$

A basis set expansion

$$\psi(x) = \sum_n \langle\phi_n|\psi(x)\rangle\phi_n$$

becomes

$$\langle x|\psi\rangle = \sum_n \langle x|\phi_n\rangle\langle\phi_n|\psi\rangle.$$

In the abstract this is just

$$|\psi\rangle = \sum_n |\phi_n\rangle\langle\phi_n|\psi\rangle$$

so

$$\sum_n |\phi_n\rangle\langle\phi_n|$$

is, for any orthonormal basis set $\{\phi_n\}$, the 'identity' operator.

This last result makes it easy to develop basis set expansions. Returning to the original experiment,

$$\Psi(t) = e^{-i\hat{H}t/\hbar}\psi_a$$

and we seek

$$\begin{aligned}\langle\phi_b|\Psi(t)\rangle &= \langle b|e^{-i\hat{H}t/\hbar}\psi_a\rangle \\ &= \sum_{m,n}\langle b|\chi_m\rangle\langle\chi_m|e^{-i\hat{H}t/\hbar}\chi_n\rangle\langle\chi_n|\psi_a\rangle \\ &= \sum_n \langle b|E_n\rangle e^{-iE_nt/\hbar}\langle E_n|a\rangle\end{aligned}$$

Finally, let us consider two different matrix representations of some operator $\hat{A}$,

$$\begin{aligned}A^{(\phi)}_{mn} =&\langle\phi_m|\hat{A}\phi_m\rangle, \\ A^{(\psi)}_{k\ell} =&\langle\psi_k|\hat{A}\psi_\ell\rangle.\end{aligned}$$

To see how they are related, we calculate

$$\begin{aligned}A^{(\psi)}_{k\ell} =&\langle\psi_k|\hat{A}\psi_\ell\rangle \\ =&\sum_{mn}\langle\psi_k|\phi_m\rangle\langle\phi_m|\hat{A}\phi_n\rangle\langle\phi_n|\psi_\ell\rangle \\ =&\sum_{mn}\langle\psi_k|\phi_m\rangle A^{(\phi)}_{mn}\langle\phi_n|\psi_\ell\rangle.\end{aligned}$$

If we define a linear transformation $\hat{S}$ by

$$\psi_\ell = \hat{S}\phi_\ell, \qquad \text{all } \ell,$$

then

$$
\begin{aligned}
\langle\phi_n|\psi_\ell\rangle =&[S]_{n\ell},\\
\langle\psi_k|\phi_m\rangle =&[\hat{S}^{-1}]_{\ell n},\\
A^{(\psi)}_{k\ell} =&\sum_{mn}[\hat{S}^{-1}]_{km}A^{(\phi)}_{mn}[S]_{n\ell}\\
=&[S^{-1}AS]_{k\ell}
\end{aligned}
$$

or

$$A^{(\psi)} = S^{-1}A^{(\phi)}S.$$

More colloquially, we say that a unitary transformation $\hat{S}$ transforms some operator $\hat{A} \to \hat{S}^{-1}\hat{A}\hat{S}$.