Quantum Dynamics

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Time-evolution Operators

We introduce the time-evolution operator $\hat{T}$,

$$|\Psi(t)\rangle = \hat{T}|\Psi(0)\rangle. \tag{1}$$

If the ket is initially normalized to unity, it must remain unitarity after time-evolution operations. Therefore, time-evolution operators must be unitary.

- Linear
- Unitary

Unitary Operators

$$|\Psi(t)\rangle = \hat{T}|\Psi(0)\rangle,$$
$$\langle\Psi(t)| = \langle\Psi(0)|\hat{T}^\dagger.$$
$$\langle\Psi(0)|\Psi(0)\rangle = 1, ,$$
$$\langle\Psi(t)|\Psi(t)\rangle = 1,$$

Then,

$$\langle\Psi(t)|\Psi(t)\rangle = \langle\Psi(0)|\hat{T}^\dagger\hat{T}|\Psi(0)\rangle = 1. \tag{2}$$

Therefore, $\hat{T}$ must be an unitary operator, $\hat{T}^\dagger\hat{T} = 1$.

Unitary Matrix & Hermitian Matrix

$$\hat{H} = \hat{H}^\dagger,$$
$$\hat{U}^{-1} = \hat{U}^\dagger.$$

If a Hermite operator $\hat{H}$ is given, we can construct the time evolution operator which is unitary

$$\hat{T} = 1 - i\epsilon\hat{H}.$$

Check that

$$\begin{aligned} \hat{T}\hat{T}^\dagger &= (1 - i\epsilon\hat{H})(1 + i\epsilon\hat{H}^\dagger) \\ &= 1 + i\epsilon\hat{H}^\dagger - i\epsilon\hat{H} + \epsilon^2\hat{H}^2 \\ &\approx 1 \end{aligned}$$

Quantum Dynamics

$$\begin{aligned}|\Psi(\epsilon)\rangle &= \hat{T}|\Psi(0)\rangle \\ &= (1 - i\epsilon\hat{H})|\Psi(0)\rangle\end{aligned}$$

$$\begin{aligned}|\Psi(\epsilon)\rangle - |\Psi(0)\rangle &= -i\epsilon\hat{H}|\Psi(0)\rangle \\ \frac{|\Psi(\epsilon)\rangle - |\Psi(0)\rangle}{\epsilon} &= -i\hat{H}|\Psi(0)\rangle \\ \frac{\partial|\Psi\rangle}{\partial t} &= -i\hat{H}|\Psi\rangle.\end{aligned}$$

Then, we have the Schrödinger equation ($\hat{H} \to \hat{H}/\hbar$):

$$i\hbar\frac{\partial|\Psi\rangle}{\partial t} = \hat{H}|\Psi\rangle. \tag{3}$$

Changing Basis & Unitary Matrix

The components of a vector depend on the choice of basis. Let us see how to change bases. The old basis vectors $|e_i\rangle$ are linear transformations of the new ones $|f_i\rangle$.

$$\begin{aligned}
|e_1\rangle &= U_{11}|f_1\rangle + U_{21}|f_2\rangle + U_{31}|f_3\rangle, \\
|e_2\rangle &= U_{12}|f_1\rangle + U_{22}|f_2\rangle + U_{32}|f_3\rangle, \\
|e_3\rangle &= U_{13}|f_1\rangle + U_{23}|f_2\rangle + U_{33}|f_3\rangle, \\
&\dots \\
|e_j\rangle &= \sum_i U_{ij}|f_i\rangle.
\end{aligned}$$

In matrix form,

$$\begin{aligned}
|A_f\rangle &= \hat{U}|A_e\rangle, \\
\hat{U}^{-1}|A_f\rangle &= |A_e\rangle,
\end{aligned}$$

where e and f represent the basis of vectors.

Changing Basis & Unitary Matrix

We introduce another operator $\hat{H}$,

$$|B_e\rangle = \hat{H}|A_e\rangle,$$

Then,

$$\begin{aligned} |B_f\rangle &= \hat{U}|B_e\rangle. \\ &= \hat{U}\hat{H}|A_e\rangle. \\ &= \hat{U}\hat{H}\hat{U}^{-1}|A_f\rangle. \end{aligned}$$

Similarity transformation is given by

$$\begin{aligned} |B_e\rangle &= \hat{H}|A_e\rangle, \\ |B_f\rangle &= \hat{U}\hat{H}\hat{U}^{-1}|A_f\rangle. \end{aligned}$$

(Advanced) Matrix Diagonalization & Unitary Matrix

We consider the eigenvector equation:

$$\hat{H}|\alpha^n\rangle = \lambda^n|\alpha^n\rangle,$$

$$\sum_j H_{ij}\alpha_j^n = \lambda^n\alpha_i^n.$$

Consider an unitary matrix U whose elements are: $U_{in} = \alpha_i^n$. Then,

$$\begin{aligned}
(U^\dagger HU)_{mn} &= \sum_{ij}(U^*)_{im}H_{ij}U_{jn} \\
&= \sum_{ij}(\alpha_i^m)^* H_{ij}\alpha_j^n \\
&= \sum_{i}(\alpha_i^m)^* \lambda^n\alpha_i^n \\
&= \lambda^n\sum_{i}(\alpha_i^m)^*\alpha_i^n = \lambda^n\delta_{mn}.
\end{aligned}$$

In conclusion, $U^\dagger HU = D_H$ where D_H is the diagonal matrix whose diagonal elements are eigenvalues of H.

(Advanced) Example of Matrix Diagonalization

$$\sigma = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}. \tag{4}$$

The eigenvectors of the matrix are

$$\frac{1}{\sqrt{2}} \begin{pmatrix} i \\ 1 \end{pmatrix}, \quad \frac{1}{\sqrt{2}} \begin{pmatrix} -i \\ 1 \end{pmatrix}. \tag{5}$$

Then, $U^\dagger \sigma U$ is

$$\frac{1}{\sqrt{2}} \begin{pmatrix} -i & 1 \\ i & 1 \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} i & -i \\ 1 & 1 \end{pmatrix} = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{6}$$

Where to go next...

Schrödinger's and Heisenberg's Pictures