Hermit and Unitary Matrix in Quantum Mechanics

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Section 1

State of the system

In physics, a state function is a quantity function that represents state of the system. Not only in quantum mechanics, and also in statistical or thermodynamics, this function is commonly treated as a system itself and used in many equations.

In quantum system, the state function is a complex valued wave function, $|\psi\rangle$. We assume that all information we want from the system can be derived from the wave function by the measurement.

The $|\rangle$ is a Dirac's braket notation. $|\rangle$ means vector and $\langle|$ means dual-vector.

Following Copenhagen interpretation, $|\psi\rangle$ yields a probability for the outcomes of measurements upon the system.

The probabilitic treatment constrains ψ in some manners. First, it must be a normalized function. Second, the measurement outcome must be *real* value.

- $\langle\psi|\psi\rangle = \int_V \psi(\mathbf{x})|\psi(\mathbf{x})\,\mathbf{dx} = 1$
- Measurement of quantity, H on the system $|\psi\rangle$ is a $\langle\psi|\hat{H}|\psi\rangle$.

Section 2

Hermit and Unitary matrix

Subsection 2.1

Unitary matrix

Let's think about there is a change, whatever it is, in the system. The $|\psi\rangle$ represent all the information of the system, so that it will be changed to $|\psi'\rangle$.

Any modification in the vector space can be represented with an *operator*, $\hat{U}$.

$$|\psi'\rangle = \hat{U}|\psi\rangle \tag{2.1}$$

Now, the modified state function also satisfies normalization, such as $\langle\psi'|\psi\rangle = \langle\psi|\psi\rangle$.

$$\begin{aligned}\langle\psi'|\psi\rangle &= \langle\hat{U}\psi||\hat{U}\psi\rangle\\ \langle\hat{U}\psi||\hat{U}\psi\rangle &= \langle\psi|\hat{U}^\dagger|\hat{U}\psi\rangle\\ \langle\psi|\hat{U}^\dagger|\hat{U}\psi\rangle &= \langle\psi|\hat{U}^\dagger\hat{U}|\psi\rangle\end{aligned}$$

we get,

$$\hat{U}^\dagger\hat{U} = \hat{I} \tag{2.2}$$

where, $\hat{I}$ is an identity operator.

That means that any state change event in the quantum system must be a unitary operator in vector space, in isolated system. With well defined basis, we can formulate the operator as matrix,

$$\begin{aligned}|\Psi\rangle \quad &= \sum c_i|\psi_i\rangle\\ [\hat{U}]_{\psi_i} &= \sum(\langle\psi_j|\hat{U}|\psi_i\rangle)|\psi_i\rangle\langle\psi_j|\end{aligned}$$

It is little bit weired that the function operation as a matrix, however, we are treating basis function that generating all functions. About the those set of functions we can find well-ordered basis, of course it does not have to be finite. Even in the infinite dimensional vector space, we can find a subspace consist of discreted index basis. Think about the Fourier series of the L periodic function. The basis functions are $\cos(\lambda_n x), n \in \mathbb{Z}_+$.

That is why the unitary matrix is essential topic in quantum computation and simulation.

2.1.1 Properties of unitary matrix

- It preserves the inner product of two vector, $\mathbf{x}, \mathbf{y}$, $\langle \mathbf{x}|\mathbf{y}\rangle = \langle U\mathbf{x}|U\mathbf{y}\rangle$
- It is a normal operator: $AA^\dagger = A^\dagger A$.
- $U^\dagger = U^{-1}$
- There exists a Hermit matrix H such that $U = \exp(iH)$.
- Eigenvalues are *unimodular* which is their norms are 1. Therefore, $|\det(U)| = 1$.

In quantum systems symulation, finding a proper unitary operation on system is important work finding equivalence but less cost unitary matrices exist in many cases.

In the property of the unitary matrix, there is $U = \exp(iH)$. It is a very familiar term in quantum mechanics; time-evolution operator.

SUBSECTION 2.2

Hermit matrix

Suppose the Hamiltonian of the system is given as H. The Schrödinger equation yields next.

$$i\hbar \frac{d}{dt}|\psi\rangle = H|\psi\rangle \tag{2.3}$$

Hamiltonian is a kind of operator of measurement for energy of the system. It means that the eigenvalues of matrix are energy of the eiegenstates. Such that

$$\hat{H}|\psi\rangle = E|\psi\rangle \tag{2.4}$$

$$\begin{aligned} \langle\psi|\hat{H}|\psi\rangle = \langle\psi||\hat{H}\psi\rangle &= \langle\hat{H}\psi||\psi\rangle && (2.5)\\ \langle\psi|\hat{H}^\dagger|\psi\rangle = E\langle\psi|\psi\rangle &= E\langle\psi|\psi\rangle && (2.6)\\ \therefore E^* &= E && (2.7) \end{aligned}$$

$E^* = E, \forall E$, the only complex value satisfying this constraint is a real value. It means that the all eigenvalues of the matrix are real value. Such matrices are called self-adjoint matrix or *Hermit matrix*.

The definition of self-adjoint matrix is

$$H^\dagger = H. \tag{2.8}$$

It is equivalence to the all eigenvalues are real condition.

We refered a Hamiltonian as an example of measurement, however, any measurement quantity operators are represented with Hermit matrices.

2.2.1 Properties of Hermite matrix

- All eigenvalues are real value.
- It is a self-adjoint matrix.
- All eigenvector having different eigenvalues are orthogonal to each other.
- Normal matrix.
- Closed under addition.
- If the two Hermite matrices are commute each other, then their product is Hermite matrix.

Additional topic: time evolution operator of Hamiltonian,