Quantum Theory of Many-Body systems in Condensed Matter (4302112) 2020

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Today's class: *Time evolution and representations*

- Schrödinger and Heisenberg pictures.
- Interaction picture.
- Time-ordering and time evolution of operators.

Time evolution: Schrödinger picture

- Schrödinger's equation (Dirac's notation):

$$i\hbar \frac{\partial |\psi_S(t)\rangle}{\partial t} = \hat{H}|\psi_S(t)\rangle \quad \Rightarrow \quad |\psi_S(t)\rangle = e^{-i\hat{H}t/\hbar}|\psi_S(0)\rangle$$

Formally:

$$e^{\hat{A}} = \mathbb{1} + \hat{A} + \frac{\hat{A}^2}{2!} + \cdots = \sum_{n=0}^{\infty} \frac{\hat{A}^n}{n!}$$

Operators in the Schrödinger picture: $\hat{A}_S = \hat{A}$ (time independent)

Time dependence of expected values:

$$\langle \hat{A} \rangle(t) = \langle \psi_S(t)|\hat{A}_S|\psi_S(t)\rangle$$

Time evolution: Heisenberg picture

Rewriting:

$$\langle \hat{A} \rangle (t) = \langle \psi_S(t) | \hat{A}_S | \psi_S(t) \rangle = \langle \psi_S(0) | e^{+i\hat{H}t/\hbar} \hat{A}_S e^{-i\hat{H}t/\hbar} | \psi_S(0) \rangle$$

States in the Heisenberg picture: $|\psi_H\rangle = |\psi_S(0)\rangle$ (time independent)

Notice that: $|\psi_H\rangle = e^{+i\hat{H}t/\hbar} |\psi_S(t)\rangle$

Operators in the Heisenberg picture: $\hat{A}_H(t) \equiv e^{+i\hat{H}t/\hbar} \hat{A}_S e^{-i\hat{H}t/\hbar}$

Notice that: $\hat{H}_H = \hat{H}_S = \hat{H}$

Time dependence of expected values: $\langle \hat{A} \rangle (t) = \langle \psi_H | \hat{A}_H(t) | \psi_H \rangle$

Time evolution: Heisenberg picture

Operators in Heisenberg Picture follow the *equation of motion*:

$$\frac{d\hat{A}_H(t)}{dt} = \frac{i}{\hbar}\left[\hat{H}, \hat{A}_S\right]_H(t) = \frac{i}{\hbar}\left[\hat{H}, \hat{A}_H(t)\right]$$

"Commutator in Heisenberg picture"

What if the operators have a explicit time dependence? $\hat{A}_t$

Schrödinger picture

$$\hat{A}_{t\,S} = \hat{A}_t$$

Heisenberg picture

$$\hat{A}_{t\,H} = e^{+i\hat{H}t/\hbar}\hat{A}_t e^{-i\hat{H}t/\hbar}$$

Equation of motion

$$\frac{d\hat{A}_{t\,H}(t)}{dt} = \frac{i}{\hbar}\left[\hat{H}, \hat{A}_{t\,S}\right]_H(t) + \left(\frac{\partial \hat{A}_{t\,S}}{\partial t}\right)_H(t)$$

Time evolution: Interaction picture

- Hamiltonian with *interaction* term: $\hat{H} = \hat{H}_0 + \hat{V}$

- Let us define the state and operator in the *interaction picture*:

$$\begin{cases} |\psi_I(t)\rangle \equiv e^{+i\hat{H}_0 t/\hbar}|\psi_S(t)\rangle \\ \hat{A}_I(t) \equiv e^{+i\hat{H}_0 t/\hbar}\hat{A}_S e^{-i\hat{H}_0 t/\hbar} \end{cases}$$

- This leads to:

$$\begin{cases} i\hbar\dfrac{\partial|\psi_I(t)\rangle}{\partial t} = \hat{V}_I(t)|\psi_I(t)\rangle \\ \dfrac{d\hat{A}_I(t)}{dt} = \dfrac{i}{\hbar}\left[\hat{H}_0, \hat{A}_I(t)\right] \end{cases}$$

Time dependence of expected values: ⇒ $\langle\hat{A}\rangle(t) = \langle\psi_I|\hat{A}_I(t)|\psi_I\rangle$

Time evolution: Interaction picture

- Ok, how to solve this equation?

$$\begin{cases} i\hbar \dfrac{\partial |\psi_I(t)\rangle}{\partial t} = \hat{V}_I(t)|\psi_I(t)\rangle \\ \hat{V}_I(t) \equiv e^{+i\hat{H}_0 t/\hbar}\hat{V}e^{-i\hat{H}_0 t/\hbar} \end{cases}$$

Notice that, in general: $\left[\hat{H}, \hat{H}_0\right] = \left[\hat{V}, \hat{H}_0\right] \neq 0$

- Formal solution (unitary propagator):

$$\begin{cases} |\psi_I(t)\rangle = \hat{U}(t, t_0)|\psi_I(t_0)\rangle \\ \hat{U}(t, t_0) = e^{\frac{i\hat{H}_0 t}{\hbar}} e^{\frac{-i\hat{H}(t-t_0)}{\hbar}} e^{\frac{-i\hat{H}_0 t_0}{\hbar}} \end{cases}$$

Propagator properties

$$\hat{U}(t,t_0) = e^{\frac{i\hat{H}_0 t}{\hbar}} e^{\frac{-i\hat{H}(t-t_0)}{\hbar}} e^{\frac{-i\hat{H}_0 t_0}{\hbar}}$$

$$\left\{\begin{array}{l}
\hat{U}(t_0,t_0) = \mathbb{1} \\
\hat{U}^\dagger(t,t_0)\hat{U}(t,t_0) = \hat{U}(t,t_0)\hat{U}^\dagger(t,t_0) = \mathbb{1} \\
\hat{U}(t_0,t)\hat{U}(t,t_0) = \mathbb{1} \\
\hat{U}(t_0,t) = \hat{U}^{-1}(t,t_0) = \hat{U}^\dagger(t,t_0) \\
\hat{U}(t_3,t_2)\hat{U}(t_2,t_1) = \hat{U}(t_3,t_1)
\end{array}\right.$$

The set of propagators form a *unitary group*.

Integral equation

$$\begin{cases} i\hbar \dfrac{\partial |\psi_I(t)\rangle}{\partial t} = \hat{V}_I(t)|\psi_I(t)\rangle \\ |\psi_I(t)\rangle = \hat{U}(t,t_0)|\psi_I(t_0)\rangle \end{cases} \Rightarrow \hat{U}(t,t_0) = \mathbb{1} - \frac{i}{\hbar}\int_{t_0}^{t} \hat{V}_I(t')\hat{U}(t',t_0)\, dt'$$

- First order: $\hat{U}(t,t_0) \approx \mathbb{1} - \dfrac{i}{\hbar}\displaystyle\int_{t_0}^{t} \hat{V}_I(t')\, dt'$
- In general: $\hat{U}(t,t_0) = \mathbb{1} - \dfrac{i}{\hbar}\displaystyle\int_{t_0}^{t} \hat{V}_I(t')\, dt' + \left(\dfrac{-i}{\hbar}\right)^2 \displaystyle\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' \hat{V}_I(t')\, \hat{V}_I(t'') + \ldots$

Notice that:

$$\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\, \hat{V}_I(t')\hat{V}_I(t'') = \frac{1}{2}\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\, \hat{V}_I(t')\hat{V}_I(t'') + \frac{1}{2}\int_{t_0}^{t} dt'' \int_{t''}^{t} dt'\, \hat{V}_I(t')\hat{V}_I(t'')$$

Time ordering operator

- Time ordering operator: $\mathcal{T}\left[\hat{A}(t_1)\hat{B}(t_2)\right] = \begin{cases} \hat{B}(t_2)\hat{A}(t_1) \text{ if } t_2 > t_1 \\ \hat{A}(t_1)\hat{B}(t_2) \text{ if } t_1 > t_2 \end{cases}$
- We can write: [redacted]

$$\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\, \hat{V}_I(t')\hat{V}_I(t'') = \frac{1}{2}\int_{t_0}^{t} dt' \int_{t_0}^{t} dt''\, \mathcal{T}\left[\hat{V}_I(t')\hat{V}_I(t'')\right]$$

$$\Rightarrow \hat{U}(t,t_0) = \mathbb{1} - \frac{i}{\hbar}\int_{t_0}^{t} \hat{V}_I(t')\, dt' + \left(\frac{-i}{\hbar}\right)^2 \frac{1}{2}\int_{t_0}^{t} dt' \int_{t_0}^{t} dt'' \mathcal{T}\left[\hat{V}_I(t')\, \hat{V}_I(t'')\right] + \ldots$$

- In general:

$$\hat{U}(t,t_0) = \mathbb{1} + \sum_{n=1}^{\infty} \frac{1}{n!}\left(\frac{-i}{\hbar}\right)^n \int_{t_0}^{t} dt_1 \cdots \int_{t_0}^{t} dt_n\, \mathcal{T}\left[\hat{V}_I(t_1)\, \hat{V}_I(t_2) \ldots \hat{V}_I(t_n)\right]$$

“Diagramatic expansion”

$$\hat{U}(t,t_0) = \mathbb{1} - \frac{i}{\hbar}\int_{t_0}^{t} \hat{V}_I(t_1)\,dt_1 + \left(\frac{-i}{\hbar}\right)^2 \frac{1}{2}\int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \mathcal{T}\left[\hat{V}_I(t_1)\,\hat{V}_I(t_2)\right] + \ldots$$

$$\hat{U}(t,t_0) =$$