Lesson 6

* * trapping system : Gross-Pitaevskii equation.
* * Feshbach resonance : tuning interaction strength.
  → Unitary limit. ←
* * Fermionic superfluidity.
* * BCS - BEC crossover *
* * low - dimension system * BKT transition
* * Unitary limit : Efimov trimer state.
  - RG analysis
  - solve S.E.
* * Bose - Hubbard model : quantum phase transition

Khomskii chapter 5; 6

张礼 葛墨林 Chapter 10.

Linear Response and Green's function.

How does one treat the general case of time dependence in 2nd quantization ?

① Schrödinger picture $\quad \partial_t H = 0$

time-independent Hamiltonian

$$i\hbar\partial_t |\psi(t)\rangle = H|\psi(t)\rangle \Rightarrow |\psi(t)\rangle = e^{-\frac{i}{\hbar}Ht}|\psi_0\rangle$$

in the following $\hbar \equiv 1$

the S - picture

$$\begin{cases} \text{States: } |\psi(t)\rangle = e^{-iHt}|\psi_0\rangle \quad \text{depend on time} \\ \text{operators: } A \text{; may or may not} \\ H \quad \text{time-independent} \end{cases} \quad (4.1)$$

② Heisenberg picture

states $|\psi_0\rangle$ time independent.

operators $A(t)$ time dependent

$$\langle \psi'(t)|A|\psi(t)\rangle = \langle \psi_0'|e^{iHt}Ae^{-iHt}|\psi_0\rangle$$

S-picture

$$\equiv \langle \psi_0'|A(t)|\psi_0\rangle$$

H-picture. (4.2)

Heisenberg picture:
- states: $|\psi_0\rangle \equiv e^{iHt}|\psi(t)\rangle = |\psi(t_0)\rangle$
- operators: $A(t) \equiv \underline{e^{iHt}Ae^{-iHt}}$

H does not depend on time

$$\dot{A}(t) = e^{iHt}(iHA - iAH + \underline{\underline{\partial_t A}})$$

$$\dot{A}(t) = i[H, A(t)] + \partial_t A \qquad (4.3)$$

③ Interaction picture

perturbation

$$H = \underline{\underline{H_0}} + \underline{\underline{V(t)}} = \underline{\underline{H_0}} + H_I$$

easy to solve

time-independent H_0; easy solve $\quad H_0|n_0\rangle = \varepsilon_{n_0}|n_0\rangle$

$V(t)$ interaction, perturbation, time-dependent or not

interaction picture
- states: $|\hat{\psi}(t)\rangle \quad \underline{e^{iH_0t}}\,\underline{|\psi(t)\rangle}_S$
- operator: $\hat{A}(t) = e^{iH_0t}Ae^{-iH_0t}$ (4.4)

have known: H_0 does not depend on time

$$i\partial_t|\hat{\psi}(t)\rangle = i\partial_t \underbrace{e^{iH_0t}|\psi(t)\rangle} = e^{iH_0t}[-H_0+H]|\psi(t)\rangle$$

$$= \underbrace{e^{iH_0t}V(t)e^{-iH_0t}}_{\hat{V}(t)}|\hat{\psi}(t)\rangle$$

$$\boxed{i\partial_t|\hat{\psi}(t)\rangle = \hat{V}(t)|\hat{\psi}(t)\rangle} \quad (4.5)$$

define time evolution operator

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

ETC:

$$\boxed{i\partial_t\hat{U}(t,t_0) = \hat{V}(t)\hat{U}(t,t_0)} \quad (4.6)$$

$$\hat{U}(t_0,t_0) = 1$$

explicit form of:

$$\hat{U}(t,t_0) = e^{iH_0t}e^{-iH(t-t_0)}e^{-iH_0t_0}$$

$$\hat{U}\cdot\hat{U}^+ = 1 \quad \text{Unitary operator}$$

Integration

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

$$\Downarrow$$

$$\hat{U}(t,t_0) = 1 + \frac{1}{i}\int_{t_0}^{t}dt'\,\hat{V}(t') + \frac{1}{i^2}\int_{t_0}^{t}dt_1\hat{V}(t_1)\int_{t_0}^{t_1}dt_2\,\hat{V}(t_2) + \cdots$$

$$\int_{t_0}^{t}dt_1\,\hat{V}(t_1)\int_{t_0}^{t_1}dt_2\,\hat{V}(t_2)$$

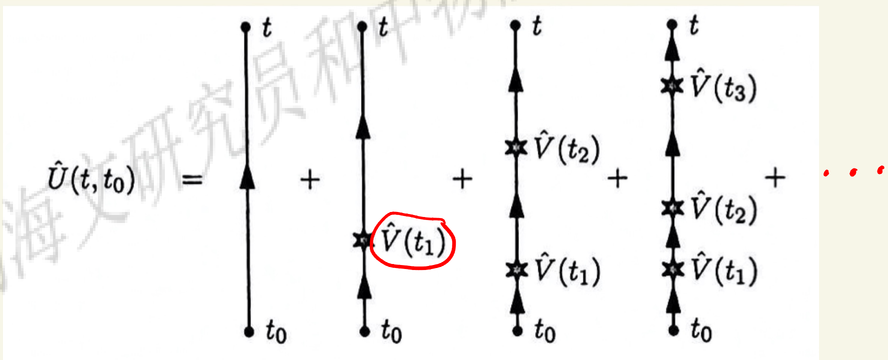
$$= \frac{1}{2}\int_{t_0}^{t}dt_1\int_{t_0}^{t}dt_2\,[\underbrace{\hat{V}(t_1)\hat{V}(t_2)\theta(t_1-t_2) + \hat{V}(t_2)\hat{V}(t_1)\theta(t_2-t_1)}]$$

$$= \frac{1}{2}\int_{0}^{t}dt_1\int_{t_0}^{t}dt_2\,T_t[\hat{V}(t_1)\hat{V}(t_2)]$$

$$\hat{U}(t,t_0) = \sum_{n=0}^{\infty} \left(\frac{1}{i}\right)^n \cdot \frac{1}{n!} \int_{t_0}^{t} dt_1 \cdots \int_{t_0}^{t} dt_n \, \underline{T_t} \left[\hat{V}(t_1) \cdots \hat{V}(t_n) \right]$$

$$\equiv \underline{T_t} \left[e^{-i \int_{t_0}^{t} \cdot \hat{V}(t') \, dt'} \right]$$ (4.7)

$\hat{U}(t,t_0)$ contains infinite-order perturbation; Feynman diagrams can be used to solve $\hat{U}(t,t_0)$.



If the perturbation $\hat{V}(t)$ is weak, we can use the first-order approximation:

$$\hat{U}(t,t_0) \simeq 1 + \frac{1}{i} \int_{t_0}^{t} dt' \, \hat{V}(t')$$

kubo formula in the linear response theory.

creation and annihilation operators in <u>Heisenberg picture</u>:

$$a_\nu^+ \longrightarrow a_\nu^+(t) = e^{iHt} a_\nu^+ a^{-iHt}$$ (4.8)

$$a_\nu \longrightarrow a_\nu(t) = e^{iHt} a_\nu e^{-iHt}$$

Bose / Fermion (anti-) commutator

$$\left[a_{\nu_1}(t_1), a_{\nu_2}^+(t_2)\right]_{F,B} = e^{iHt_1} a_{\nu_1} e^{-iH(t_1-t_2)} a_{\nu_2}^+ e^{-iHt_2}$$

$$\pm e^{iHt_2} a_{\nu_2}^+ e^{-iH(t_1-t_2)} a_{\nu_1} e^{-iHt_1}$$??

example: consider a time-independent Hamiltonian H

$$H = \sum_\nu \varepsilon_\nu \overset{\text{S-picture}}{a_\nu^\dagger a_\nu} = \sum_\nu \varepsilon_\nu \overset{\text{H-picture}}{a_\nu^\dagger(t)\, a_\nu(t)}$$

H-picture

$$\dot{a}_\nu(t) = i[H, a_\nu(t)] = i e^{iHt} \sum_{\nu'} \varepsilon_{\nu'} [a_{\nu'}^\dagger a_{\nu'}, a_\nu] e^{-iHt}$$

$$= -i \varepsilon_\nu e^{iHt} a_\nu e^{-iHt} = -i \varepsilon_\nu a_\nu(t)$$

$$a_\nu(t) = e^{-i\varepsilon_\nu t} a_\nu$$

$$a_\nu^\dagger(t) = e^{i\varepsilon_\nu t} a_\nu^\dagger$$

$$[a_{\nu_1}(t_1), a_{\nu_2}^\dagger(t_2)]_{F,B} = e^{i\varepsilon_{\nu_1}(t_1 - t_2)} \delta_{\nu_1 \nu_2} \qquad (4.9)$$

Consider a trivial extension of interaction picture.

$$H = H_0 + \underbrace{\gamma H_0}_{H_1} \qquad \gamma \ll 1$$

H_0 basis $\{|\nu\rangle\}$, ε_ν

Interaction picture: $|\hat{\nu}(t)\rangle = e^{i\varepsilon_\nu t} \overset{\text{S-picture}}{|\nu(t)\rangle}$

$$|\nu(t)\rangle = e^{-i(1+\gamma)\varepsilon_\nu t} |\nu\rangle$$

$$\underset{\text{I-picture}}{|\hat{\nu}(t)\rangle} = e^{-i\gamma\varepsilon_\nu \cdot t} \underset{\text{H-picture}}{|\nu\rangle} \qquad (4.10)$$

Consider a time-independent V, but Coulomb-like interaction

$$H = H_0 + V = \sum_{\nu'} \varepsilon_{\nu'} a_{\nu'}^\dagger a_{\nu'} + \frac{1}{2} \sum_{\nu_1 \nu_2 q} V_q a_{\nu_1+q}^\dagger a_{\nu_2-q}^\dagger a_{\nu_2} a_{\nu_1}$$

$$\dot{a}_\nu(t) = i[H, a_\nu(t)] = -i\varepsilon_\nu a_\nu(t) \checkmark \qquad (4.11)$$

$$+ \frac{i}{2}\sum_{\nu_1 \nu_2 q} V_q \underbrace{[a^\dagger_{\nu_1+q}\, a^\dagger_{\nu_2-q},\, a_\nu(t)]\cdot a_{\nu_2}\cdot a_{\nu_1}}_{\text{three - operators}}$$

approximation: self-consistent; turcation;

$\boxed{\text{equation of motion.}}$

Correlation function; Green's function.

kubo formula

retarded function: $t > t'$ Bose-type

$$\hookrightarrow C^R_{AB}(t,t') = -i\,\theta(t,t')\,\langle [A(t), B(t')] \rangle_0 \qquad (4.12)$$

$C^A_{AB}(t,t')$

Fermion-type

$$C^R_{AB}(t,t') = -i\,\theta(t,t')\,\langle \{A(t), B(t')\} \rangle \qquad (4.13)$$

$A(t)$, $B(t)$; Heisenberg picture.

Baym; Koldysh;

$\langle \cdot \rangle$ thermal average

$$\langle A(t) B(t') \rangle = \frac{1}{Z} \mathrm{Tr}\left[e^{-\beta H} e^{iHt} A e^{-iHt} e^{iHt'} B e^{-iHt'}\right]$$

$$= \frac{1}{Z} \mathrm{Tr}\left[e^{-\beta H} e^{iH(t-t')} A e^{-iH(t-t')} B\right] \qquad (4.14)$$

Hamiltonian do not depends on time; $\langle A(t) B(t') \rangle \sim t-t'$

Since $C^R_{AB}(t,t') \equiv C^R_{AB}(t-t')$

Fourier transform :

$$C^R_{AB}(\omega) = \int_{-\infty}^{\infty} dt\, e^{i\omega t}\, \underline{\underline{C^R_{AB}(t)}}$$

4.15

$C^R_{AB}(t)$; usually $t \to \infty$, $C^R_{AB}(t) \to 0$

however : $C^R_{AB}(t) \propto \exp[i \Sigma t]$

$t \to \infty$, $C^R_{AB}(t)$ oscillation.

$0^+ = \zeta$

$$C^R_{AB}(\omega) = \int_{-\infty}^{\infty} dt\, e^{i(\omega + i0^+)t}\, C^R_{AB}(t)$$

$e^{-0^+ t} \to 0$

$t \to \infty$

$\omega \longrightarrow \omega + i0^+$

$$C^A_{AB}(t,t') = i\,\theta(t'-t)\,\langle [A(t), B(t')]_{F,B} \rangle$$

B ← commutator

F ← anti-commutator

$\omega \to \omega - i0^+$

Interaction picture : $H = H_0 + V(t)$

$$i\partial_t |\hat{\psi}(t)\rangle = \hat{V}(t)\, |\hat{\psi}(t)\rangle$$

$$\hat{V}(t) = e^{iH_0 t}\, V(t)\, e^{-iH_0 t}$$

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

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

$$\hat{U}(t,t_0) = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{1}{i}\right)^n \int_{t_0}^{t} dt_1 \cdots \int_{t_0}^{t} dt_n\, T_t[\hat{V}(t_1) \cdots \hat{V}(t_n)]$$

↑ Feynman diagrams.

first order approximation :

$$\hat{U}(t,t_0) = 1 + \frac{1}{i}\int_{t_0}^{t} dt'\, \hat{V}(t_1)$$

Linear Response theory and kubo formula.

expectation of what?

$$\underset{H_0}{\langle A_0 \rangle} + \langle \delta A \rangle \Leftarrow H_0 + H'$$

$\langle \delta A^2 \rangle$

$$\langle A_0 \rangle \longleftrightarrow H_0$$

physical quantity.

what is the relation between $\langle \delta A \rangle$ and H'

H' weak perturbation.

linear response $\leftarrow$
- charge susceptibility.
- spin susceptibility.
- conductivity.

the general kubo formula.

time independent H_0 in thermodynamic equilibrium

operator A : physical quantity.

$$\langle A \rangle = \frac{1}{Z_0} \mathrm{Tr}[\rho A] = \frac{1}{Z_0} \sum_n \langle n | A | n \rangle e^{-\beta E_n}$$

$$\rho = \sum_n |n\rangle\langle n| e^{-\beta E_n}$$

$$H(t) = H_0 + H'(t)\,\theta(t - t_0)$$

$H'(t)$ weak perturbation, influence the eigenstates but not eigenvalues.

s-picture.

$$\langle A \rangle (t) = \frac{1}{Z_0} \sum_n \langle n(t) | A | n(t) \rangle e^{-\beta E_n} \qquad (4.16)$$

$$i \partial_t |n(t)\rangle = H(t) |n(t)\rangle$$

$$|\hat{n}(t)\rangle = e^{iH_0 t} |n(t)\rangle$$

S-picture $\Rightarrow |n(t)\rangle = e^{-iH_0 t}\, |\hat{n}(t)\rangle \leftarrow$ I-picture

$$= e^{-iH_0 t}\, \hat{U}(t,t_0)\, \underbrace{|\hat{n}(t_0)\rangle}_{|n\rangle}$$

$$|n(t)\rangle = e^{-iH_0 t}\, \hat{U}(t,t_0)\, |n\rangle \qquad \hat{U}(t,t_0) = 1 - i\int_{t_0}^{t} dt'\, \hat{H}'(t')$$

$$\langle A\rangle(t) = \frac{1}{Z_0}\sum_n \langle n|\, \underbrace{\hat{U}^+(t,t_0)}_{1}\, \underbrace{e^{iH_0 t}\, A\, e^{-iH_0 t}}_{=\hat{A}(t)}\, \underbrace{\hat{U}(t,t_0)}_{1}|n\rangle \qquad e^{-\beta E_n}$$

$$= \langle A\rangle_0 - i\int_{t_0}^{t} dt' \sum_n e^{-\beta E_n} \langle n|\, \underbrace{\hat{A}(t)\,\hat{H}'(t')}_{\hat{U}} - \underbrace{\hat{H}'(t')\,\hat{A}(t)}_{\hat{U}^+}|n\rangle$$

ETC

$$= \langle A\rangle_0 - i\int_{t_0}^{t} dt' \left\langle\left[\hat{A}(t),\, \hat{H}'(t')\right]\right\rangle_0$$

H_0 thermal expectation

$$\delta\langle A\rangle(t) = \langle A\rangle(t) - \langle A\rangle_0$$

$$= -i\int_{t_0}^{t} dt' \left\langle\left[\hat{A}(t),\, \hat{H}'(t')\right]\right\rangle_0 \qquad (4.17)$$

$$= \int_{t_0}^{\infty} dt'\, C^R_{AH'}(t,t') \qquad \theta(t,t') \begin{cases} 1 & t>t' \\ 0 & t<t' \end{cases}$$

Correlation function

$$C^R_{AH'}(t,t') = -i\,\underbrace{\theta(t,t')}_{\boxed{t>t'}} \left\langle\left[\hat{A}(t),\, \hat{H}'(t')\right]\right\rangle_0 \qquad (4.18)$$

H_0 basis

Linear response of kubo formula.

$\hat{A}(t)$; $\hat{H}'(t)$ explicit form :

external perturbation

S-picture. $H_B'(t') = B f(t')$ $\qquad$ B time-independent

$f(t)$ is not operator

$$C^R_{AH'}(t,t') = C^R_{AB}(t-t') f(t')$$

$$\delta A(t) = \int_{t_0}^{\infty} dt' \, C^R_{AB}(t-t') f(t') \qquad (4.19)$$

$\Downarrow$ convolution form.

$$\delta A(\omega) = C^R_{AB}(\omega) f(\omega)$$

generalization

$$H_B'(t) = \sum_\alpha \int d\vec{r} \, B^\alpha(\vec{r}) f^\alpha(r,t)$$

$$\delta A(\omega) = \sum_\alpha \int d\vec{r} \, C^R_{AB^\alpha(r)}(\omega) f^\alpha(r,\omega) \qquad (4.20)$$

$$H'(t) = H' \theta(t - t_0)$$

$\langle A \rangle_{eq} = A_0$ $\qquad t_0 \qquad \delta \langle A \rangle (t)$

$$\sim \langle [A(t), H'(t')] \rangle_{eq}$$

Kubo formula for conductivity.

H is time-independent

$$I_e^{\alpha}(\vec{r}, t) = \int dt' \int d\vec{r}' \sum_{\beta} \sigma^{\alpha\beta}(\vec{r}, \vec{r}', \underline{t-t'}) \cdot E_{ext}^{\beta}(\vec{r}', t')$$

4.21

$$I_e^{\alpha}(r, \omega) = \int dr' \sum_{\beta} \sigma^{\alpha\beta}(r, r', \omega) E^{\beta}(r', \omega)$$

$$H = \frac{1}{2m} \sum_{\sigma} \int dr\, \Psi_\sigma^{+}(r) \left[\frac{\hbar}{i} \nabla_r - q\vec{A} \right]^2 \Psi_\sigma(r)$$

electron system

$q = -e$

$$H = H_0 + \delta H$$

$$\delta H = -q \int dr\, \vec{J} \cdot \vec{A} \Rightarrow \vec{J} = \frac{\delta H}{\delta A} \cdot \frac{1}{-q}$$

$$\Delta H = \int dr\, -q \cdot \frac{\hbar}{i \cdot 2m} \left[\Psi_\sigma^{+}(r) (\nabla \Psi_\sigma(r)) - (\nabla \Psi_\sigma^{+}(r)) \Psi_\sigma(r) \right] \cdot \vec{A}$$

$$+ \int \frac{q^2}{2m} A^2 \Psi_\sigma^{+}(r) \Psi_\sigma(r)\, dr$$

$$J_{tot}(r,t) = J(t) - \frac{q}{m} A(r,t)\, \rho(r)$$

$$J_\sigma(r) = J_\sigma^{\nabla}(r) + J_\sigma^{A}(r)$$

4.22

current ← current

$$J_\sigma^{\nabla}(r) = \frac{\hbar}{2mi} \left[\Psi_\sigma^{+}(r) (\nabla \Psi_\sigma(r)) - (\nabla \Psi_\sigma^{+}(r)) \Psi_\sigma(r) \right]$$

← diamagnetic current

$$J_\sigma^{A}(r) = -\frac{q}{m} A(r)\, \underline{\Psi_\sigma^{+}(r) \Psi_\sigma(r)}$$

momentu Representation.

$$J_\sigma^{v}(r) = \frac{\hbar}{mV}\sum_{k,q}\left(\vec{k} + \frac{\vec{q}}{2}\right) e^{i\vec{q}\vec{r}}\, a^{+}_{\vec{k},\sigma}\, a_{\vec{k}+\vec{q},\sigma} \qquad (4.23)$$

$$J_\sigma^{A}(r) = \frac{-q}{mV}\, A(r) \sum_{\vec{k},\vec{q}} e^{i\vec{q}\vec{r}}\, a^{+}_{\vec{k}\sigma}\, a_{\vec{k}+\vec{q},\sigma}$$

electron

$$H'(t) = e\int dr\, J^{\beta}_{tot}\cdot A^{\beta}$$ ✓

velocity

$$J_{tot}(r,t) = \underbrace{J(t)}_{①} - \underbrace{\frac{q}{m}A(r,t)}_{②}\,\rho(r) \qquad (4.24)$$

$$= J(t) + \frac{e}{m}A(r,t)\,\rho(r)$$

electron current : $I(t) \equiv -e\, J_{tot}(t)$

$$I_e(t) = -e\,J(t) - \frac{e^2}{m}A(r,t)\,\rho(r)$$

velocity

①velocity current ②diamagnetic current

$$\langle \delta I_e\rangle(t) = -e\langle J\rangle(t) - \underbrace{\frac{e^2}{m}A(r,t)\langle\rho(r)\rangle_0}_{②}$$

$$\langle J\rangle(t) = \int dr'\int dt' \sum_{\beta} C^{R}_{J(r)H'(t')}(t,t')$$

$$H'(t') = e\int dr\left[\vec{J}(t') + \frac{e}{m}\vec{A}(r,t')\rho(r)\right]\cdot\vec{A}(r,t')$$

$$= e\int dr'\int dt' \sum_{\beta} C^{R}_{J(r)J^{\beta}(r')}(t-t')\cdot A^{\beta}(r',t') \qquad (4.26)$$

$$\langle \delta I_e \rangle(t) = -e^2 \int dr' \int dt' \sum_\beta C^R_{J(r) J^\beta(r')}(t-t')\, A^\beta(r',t')$$

$$- \frac{e^2}{m} A(r,t) \langle \rho(r) \rangle_0$$

we know $\partial_t A(r,t) = E(r,t) \Rightarrow A(r,\omega) = \dfrac{E(r,\omega)}{i\omega}$ (4.27)

frequency domain

$$\langle \delta I_e^\alpha \rangle(\omega) = -e^2 \int dr' \sum_\beta C^R_{J^\alpha(r) J^\beta(r')}(\omega)\, A^\beta(r',\omega)$$

$$- \frac{e^2}{m} A^\alpha(r,\omega) \langle \rho(r) \rangle_0$$

$$= \frac{ie^2}{\omega} \int dr' \sum_\beta C^R_{J^\alpha(r) J^\beta(r')}(\omega)\, E^\beta(r',\omega)$$

$$+ \frac{ie^2}{m\omega} n(r) E^\alpha(r,\omega)$$

$$I_e^\alpha(r,\omega) = \int dr' \sum_\beta \sigma^{\alpha\beta}(r,r',\omega)\, E^\beta(r',\omega)$$

$$\boxed{\begin{aligned} \sigma^{\alpha\beta}(r,r',\omega) &= \frac{ie^2}{\omega} \Pi^R_{\alpha\beta}(r,r',\omega) \quad ① \\ &+ \frac{ie^2 n(r)}{m\omega} \delta(r-r')\, \delta_{\alpha\beta} \quad ② \end{aligned}}$$ (4.28)

① $\Pi^R_{\alpha\beta}(r,r',t-t') = C^R_{J_0^\alpha(r) J_0^\beta(r')}(t-t')$