

Perturbation theory & Feynman diagrams - part 2

① Overview

- motivation: $\hat{H} = \hat{H}_0 + \hat{V}$

$$\hat{H}_0 = \sum_{kG} \varepsilon_k \hat{c}_{kG}^+ \hat{c}_{kG} \quad \text{non-interacting particles (electrons in a single band)}$$

$$\hat{V} = \frac{1}{2} \sum_{kk'qGG'} V_{qG} \hat{c}_{k+qG}^+ \hat{c}_{k'-qG'}^+ \hat{c}_{k'G'} \hat{c}_{kG} \quad \text{pair interaction (Coulomb interaction)}$$

start with \hat{H}_0 and include \hat{V} perturbatively up to infinite order

- non-stationary perturbation theory

Dyson series

$$|\tilde{\psi}(t)\rangle = \left[\sum_{n=0}^{\infty} \left(-\frac{i}{\hbar} \right)^n \int_0^t dt_1 \int_0^{t_1} dt_2 \dots \int_0^{t_{n-1}} dt_n \tilde{V}(t_1) \tilde{V}(t_2) \dots \tilde{V}(t_n) \right] |\tilde{\psi}(0)\rangle$$

interaction picture

$$|\tilde{\psi}(t)\rangle = e^{\frac{i}{\hbar} \hat{H}_0 t} |\psi(t)\rangle \quad \tilde{V}(t) = e^{\frac{i}{\hbar} \hat{H}_0 t} \hat{V}(t) e^{-\frac{i}{\hbar} \hat{H}_0 t}$$

- thermal propagators

$$G(\tau, \tau') = -\frac{1}{\hbar} \frac{\text{Tr} [e^{-\beta \hat{H}} T \{ \hat{A}(\tau) \hat{B}(\tau') \}] }{\text{Tr} [e^{-\beta \hat{H}}]}$$

Heisenberg operators

$$\hat{A}(\tau) = e^{\frac{i}{\hbar} \hat{H}} \hat{A} e^{-\frac{i}{\hbar} \hat{H}}$$

interaction picture

$$\tilde{A}(\tau) = e^{\frac{i}{\hbar} \hat{H}_0} \hat{A} e^{-\frac{i}{\hbar} \hat{H}_0}$$

- Dyson expansion of the thermal propagator

$$G(\tau \geq 0) = -\frac{1}{\hbar} \frac{\langle T \{ U(t_\beta) \hat{c}_A(\tau) \hat{c}_B^\dagger(0) \} \rangle_0}{\langle U(t_\beta) \rangle_0}$$

\leftarrow averages for a non-interacting system

$$U(t_\beta) = \hat{I} + \frac{1}{1!} \left(-\frac{1}{\hbar}\right)^1 \int_0^{t_\beta} d\tau_1 \tilde{V}(\tau_1) + \dots$$

$$G(\tau \geq 0) = -\frac{1}{\hbar} \frac{\langle T \left\{ \sum_{n=0}^{\infty} \left(-\frac{1}{\hbar}\right)^n \frac{1}{n!} \int_0^{t_\beta} d\tau_1 \int_0^{t_\beta} d\tau_2 \dots \int_0^{t_\beta} d\tau_n \tilde{V}(\tau_1) \tilde{V}(\tau_2) \dots \tilde{V}(\tau_n) \tilde{A}(\tau) \tilde{B}(0) \right\} \rangle_0}{\langle T \left\{ \sum_{n=0}^{\infty} \left(-\frac{1}{\hbar}\right)^n \frac{1}{n!} \int_0^{t_\beta} d\tau_1 \int_0^{t_\beta} d\tau_2 \dots \int_0^{t_\beta} d\tau_n \tilde{V}(\tau_1) \tilde{V}(\tau_2) \dots \tilde{V}(\tau_n) \right\} \rangle_0}$$

$\tilde{V}, \tilde{A}, \tilde{B}$ expressed using c^\dagger, c

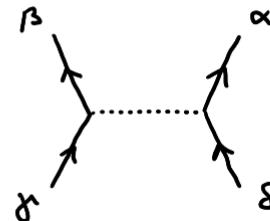
Wick's theorem

products of non-interacting G_0

• Feynman diagrams

$$\tilde{V}(\tau) = \frac{1}{2} \sum_{\alpha\beta\gamma\delta} V_{\alpha\beta\gamma\delta} \hat{c}_\alpha^+(\tau^+) \hat{c}_\beta^+(\tau^+) \hat{c}_\gamma(\tau^-) \hat{c}_\delta(\tau^-)$$

↑ ↑ ↑ ↑
Labels of single-particle states



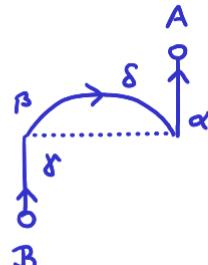
useful to keep track of the terms in the perturbation series

$$g \sim -\frac{1}{\hbar} \langle T \{ \hat{c}_A(\tau) \hat{c}_B^+(0) \} \rangle \quad \leftarrow \text{Heisenberg} \quad \downarrow \text{interaction picture}$$

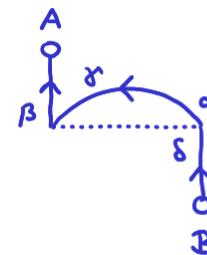
$$g \sim \frac{1}{...} [... + \langle T \{ \hat{c}_A(\tau) \hat{c}_\alpha^+(\tau_1^+) \hat{c}_\beta^+(\tau_1^+) \hat{c}_\gamma(\tau_1^-) \hat{c}_\delta(\tau_1^-) \hat{c}_B^+(0) \} \rangle_0 + ...]$$

Hartree-Fock terms

$$c_A c_\alpha^+ c_\beta^+ c_\gamma c_\delta c_B^+$$



τ
 τ_1
 $\tau' = 0$



$$c_A c_\alpha^+ c_\beta^+ c_\gamma c_\delta c_B^+$$

GOAL 1: reduction of the series (combinatorial explosion of terms with increasing n)

$$g \sim \frac{\left(\begin{array}{c} \text{Diagram} \\ + \frac{1}{1!} \left(-\frac{1}{\hbar} \right)^1 \frac{1}{2} V \left[\text{Diagram} \dots \text{Diagram} \right] + \dots \end{array} \right)}{1 + \frac{1}{1!} \left(-\frac{1}{\hbar} \right)^1 \frac{1}{2} V \left[\text{Diagram} \dots \text{Diagram} + \text{Diagram} \right] + \dots}$$

GOAL 2: diagrammatic rules - how to convert a diagram into an expression

$$n=1 \text{ in the numerator : } \langle T \left\{ \hat{c}_A(\tau) \hat{c}_\alpha^+(\tau_1^+) \hat{c}_\beta^+(\tau_1^+) \hat{c}_\delta(\tau_1) \hat{c}_\gamma(\tau_1) \hat{c}_B^+(0) \right\} \rangle_o$$

$$\begin{aligned} & c_A c_\alpha^+ c_\beta^+ c_\delta c_\gamma c_B^+ \\ & \text{Diagram: A vertical line from } \tau' = 0 \text{ to } \tau \text{ with two horizontal segments labeled } \alpha \text{ and } \beta. \text{ A curved arrow labeled } \delta \text{ connects } \alpha \text{ and } \beta. \\ & -\frac{1}{\hbar} \quad \left(-\frac{1}{\hbar} \right)^1 \frac{1}{1!} \int_0^\hbar d\tau_1 \quad \sum_{\alpha\beta\gamma\delta} \frac{1}{2} V_{\alpha\beta\gamma\delta} \\ & \pm g_o(A, \alpha, \tau - \tau_1) \quad g_o(\delta, \beta, 0^-) \\ & \qquad \qquad \qquad g_o(\gamma, B, \tau_1 - \tau') \end{aligned}$$

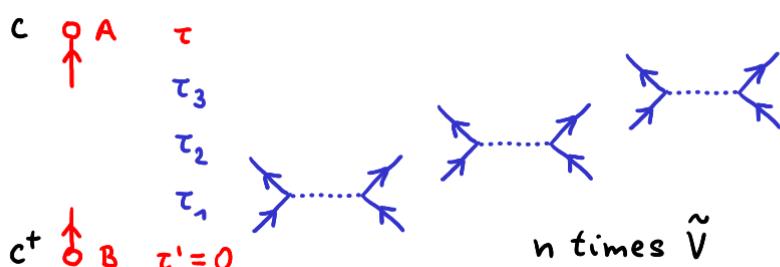
② Reduction of the number of diagrams ($\infty \rightarrow \text{smaller } \infty$)

$$g \sim \frac{\begin{array}{c} \text{Diagram with } n \text{ vertices} \\ + \frac{1}{1!} \left(-\frac{1}{h}\right)^1 \frac{1}{2} V \left[\text{Diagram with } n+1 \text{ vertices} + \text{Diagram with } n+1 \text{ vertices} + \dots \right] \end{array}}{1 + \frac{1}{1!} \left(-\frac{1}{h}\right)^1 \frac{1}{2} V \left[\text{Diagram with } n+1 \text{ vertices} + \text{Diagram with } n+1 \text{ vertices} \right] + \dots}$$

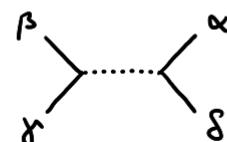
- cancellation of disconnected diagrams

numerator of single-particle propagator

$$\langle T \left\{ \sum_{n=0}^{\infty} \left(-\frac{1}{h}\right)^n \frac{1}{n!} \int_0^{t_B} d\tau_1 \int_0^{t_B} d\tau_2 \dots \int_0^{t_B} d\tau_n \tilde{V}(\tau_1) \tilde{V}(\tau_2) \dots \tilde{V}(\tau_n) \hat{c}_A(\tau) \hat{c}_B^\dagger(\tau) \right\} \rangle$$



$$\tilde{V} = \sum V c_\alpha^\dagger c_\beta^\dagger c_\gamma c_\delta$$



A and B always connected by a **backbone** of the diagram - continuous ↑ line

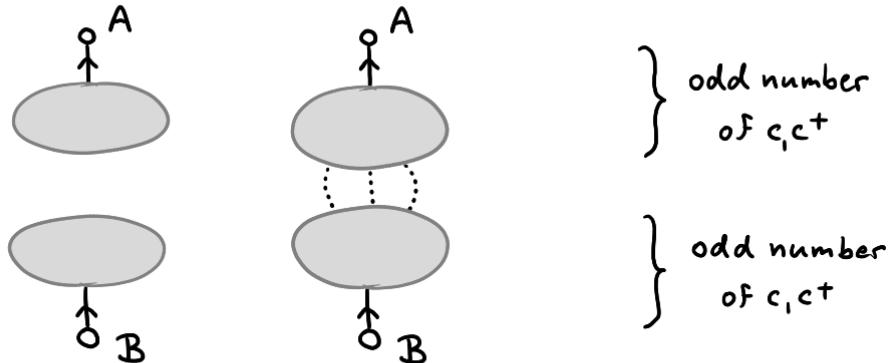
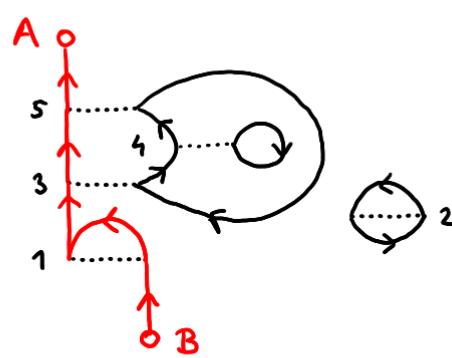
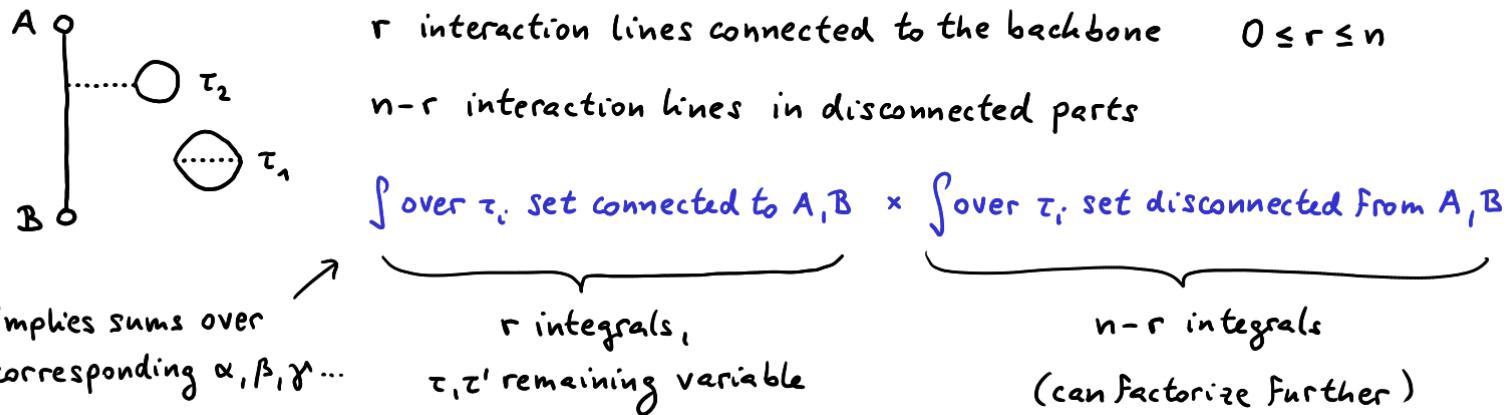


diagram of order $n \rightarrow n$ interaction lines $> \dots <$



distribution into r and $n-r$ lines can be done in $\binom{n}{r}$ ways

$$\text{G numerator} = \sum_{n=0}^{\infty} \frac{1}{n!} \left(-\frac{1}{2t}\right)^n \quad [\text{all diagrams with } n \text{ lines}]$$

From pair \tilde{V}

$$\sum_{n=0}^{\infty} \frac{1}{n!} \left(-\frac{1}{2t}\right)^n \sum_{r=0}^n \binom{n}{n-r} \begin{bmatrix} \text{diagrams with } r \text{} \\ \text{lines connected to AB} \end{bmatrix} \begin{bmatrix} \text{disconnected diagrams} \\ \text{containing } n-r \text{ lines} \end{bmatrix}$$

$\frac{n!}{(n-r)! r!}$

r integrals over τ_i
and corresponding $\sum_{\alpha \dots}$

$n-r$ integrals over τ_i .

$$\sum_{n=0}^{\infty} \sum_{r=0}^n \frac{1}{r!} \left(-\frac{1}{2t}\right)^r \begin{bmatrix} \text{diagrams with } r \text{} \\ \text{lines connected to AB} \end{bmatrix} \frac{1}{(n-r)!} \left(-\frac{1}{2t}\right)^{n-r} \begin{bmatrix} \text{disconnected diagrams} \\ \text{containing } n-r \text{ lines} \end{bmatrix}$$

$$\sum_{m=0}^{\infty} \frac{1}{m!} \left(-\frac{1}{2t}\right)^m \begin{bmatrix} \text{diagrams with } m \text{} \\ \text{lines connected to AB} \end{bmatrix} \sum_{m'=0}^{\infty} \frac{1}{m'!} \left(-\frac{1}{2t}\right)^{m'} \begin{bmatrix} \text{disconnected diagrams} \\ \text{containing } m' \text{ lines} \end{bmatrix}$$

denominator

$$\rightarrow g(z \geq 0) = -\frac{1}{t} \sum_{n=0}^{\infty} \frac{1}{n!} \left(-\frac{1}{2t}\right)^n \begin{bmatrix} \text{diagrams with } n \dots \\ \text{lines connected to AB} \end{bmatrix}$$

- cancellation of $\frac{1}{n!}$

permuting $\tau_1 \dots \tau_n$ only changes the vertical stacking of time labels

$\rightarrow n!$ equivalent contributions $\rightarrow \frac{1}{n!}$ cancelled

Example:

$$\frac{1}{2!} \left(\begin{array}{c} \text{Diagram with two lines, labels } \tau_1, \tau_2 \\ \text{Diagram with two lines, labels } \tau_2, \tau_1 \end{array} \right) = \begin{array}{c} \text{Diagram with two lines, labels } \tau_1, \tau_2 \\ \text{ordered} \end{array}$$

- cancellation of $\frac{1}{2}$

each interaction line can be used in two orientations \rightarrow compensation of $\frac{1}{2^n}$

$$\frac{1}{2} V_q \left(\begin{array}{c} \text{Diagram with one line, label } \tau_1 \\ \text{Diagram with one line, label } \tau_2 \end{array} \right) = V_q \begin{array}{c} \text{Diagram with one line, label } \tau_1 \end{array}$$

$$\rightarrow G(\tau \geq 0) = -\frac{1}{\hbar} \sum_{n=0}^{\infty} \left(-\frac{1}{\hbar}\right)^n \left[\begin{array}{l} \text{topologically inequivalent diagrams with} \\ n \dots \text{interaction lines connected to A, B} \end{array} \right]$$

up to second order:

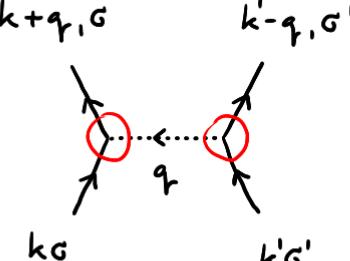
$$G(\tau \geq 0) = \begin{array}{c} n=0 \\ \text{---|---} \\ \text{---|---} \end{array} + \begin{array}{c} n=1 \\ \text{---|---} \\ \text{---|---} \\ \text{---|---} \end{array} + \begin{array}{c} n=1 \\ \text{---|---} \\ \text{---|---} \\ \text{---|---} \\ \text{---|---} \end{array} + \dots$$

③ Conservation of momentum (+ spin)

- translationally invariant system
→ momentum conservation

- spin isotropic system
→ spin conservation

- conserving interaction - Coulomb interaction



$$V = \frac{1}{2} \sum_{kk'q,GG'} V_q \hat{c}_{k+q,G}^+ \hat{c}_{k'-q,G'}^+ \hat{c}_{k',G'}^- \hat{c}_{k,G}^- \quad V_q = \frac{1}{\Omega} \frac{e^2}{\epsilon_0 q^2}$$

conservation - momentum: $k + k' = (k+q) + (k'-q)$

spin: $G \rightarrow G \quad G' \rightarrow G'$

internal momentum transfer q associated with
no transfer of spin through the Coulomb line

single-particle propagator

$$G_0(k, \tau) = -\frac{1}{\hbar} \langle T \{ \hat{c}_{k,G}(z) \hat{c}_{k,G}^+(0) \} \rangle$$

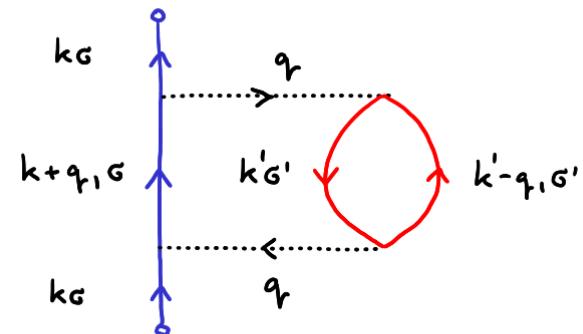
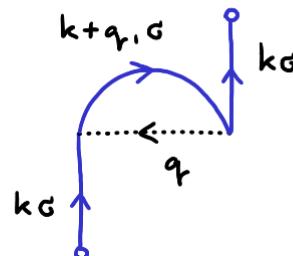
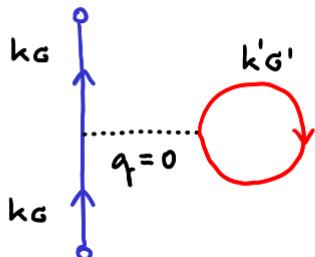
(the same for G)

- rules for the momentum and spin "flow" through the diagram:

- 1) propagators keep their momentum/spin
- 2) momentum and spin conserved at each vertex

$$g \sim \langle T \{ \hat{c}_{kG}(z) \hat{c}_{kG}^+(z') \} \rangle$$

$$V = \frac{1}{2} \sum_{kk'qGG'} V_{q_f} \hat{c}_{k+q,G}^+ \hat{c}_{k'-q,G'}^+ \hat{c}_{k'G'} \hat{c}_{kG}$$



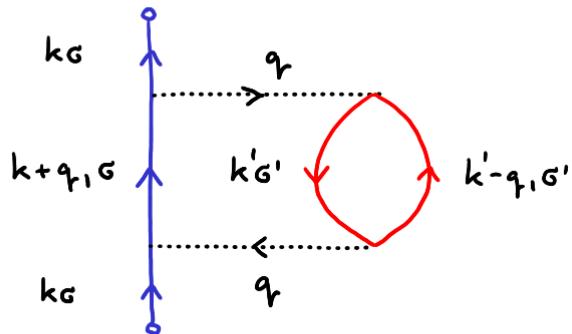
$$\sum_{k'G'} V_{q_f=0} G_{kG} G_{kG} G_{k'G'}$$

$$\sum_q V_{q_f} G_{kG} G_{k+q,G} G_{kG}$$

$$\sum_{q,k'G'} V_{q_f}^2 G_{kG} G_{k+q,G} G_{kG} G_{k'G'} G_{k'-q,G'}$$

- Free momenta and spins to be summed over

④ Conversion to Matsubara representation

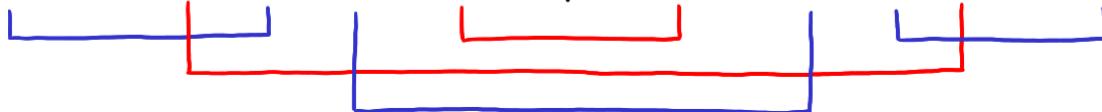


τ
 τ_1
 τ_2
 $\tau' = 0$

- $\text{t}_\hbar G(k, \tau)$ contains

$$\left(-\frac{1}{\text{t}_\hbar}\right)^2 \int_0^{\text{t}_\hbar \beta} d\tau_1 \int_0^{\text{t}_\hbar \beta} d\tau_2 \sum_{q k' G'} \langle \dots \rangle_0$$

$$\langle \dots \rangle_0 = \langle T \{ c_{k_G}(\tau) (V_{q_r} c_{k'_G'}^+ c_{k_G}^+ c_{k+q_r, G} c_{k'-q_r, G'}) \}_{\tau_1} (V_{-q_r} c_{k'-q_r, G'}^+ c_{k+q_r, G}^+ c_{k_G} c_{k'_G'}) \}_{\tau_2} c_{k_G}^+(0) \}$$



$$= V^2 \langle T \{ c_{k_G}(\tau) c_{k_G}^+(\tau_1) \} \rangle_0 \langle T \{ c_{k+q_r, G}(\tau_1) c_{k+q_r, G}^+(\tau_2) \} \rangle_0 \langle T \{ c_{k_G}(\tau_2) c_{k_G}^+(0) \} \rangle_0 \times$$

$$\times \langle T \{ c_{k'_G'}^+(\tau_1) c_{k'_G'}(\tau_2) \} \rangle_0 \langle T \{ c_{k'-q_r, G'}(\tau_1) c_{k'-q_r, G'}^+(\tau_2) \} \rangle_0$$

$$= V^2 [-\text{t}_\hbar G_o(k, \tau - \tau_1)] [-\text{t}_\hbar G_o(k+q_r, \tau_1 - \tau_2)] [-\text{t}_\hbar G_o(k, \tau_2)] [-\text{t}_\hbar (-) G_o(k', \tau_2 - \tau_1)] [-\text{t}_\hbar G_o(k'-q_r, \tau_1 - \tau_2)]$$

$-\hbar G(k, \tau)$ contains

$$\left(-\frac{1}{\hbar}\right)^2 \int_0^{\hbar\beta} d\tau_1 \int_0^{\hbar\beta} d\tau_2 \sum_{qk'g'} V_q^2 [-\hbar g_o(k, \tau - \tau_1)] [-\hbar g_o(k+q, \tau_1 - \tau_2)] [-\hbar (-) g_o(k', \tau_2 - \tau_1)] [-\hbar g_o(k'-q, \tau_1 - \tau_2)]$$

- Matsubara coefficients $-G(k, iE) = \frac{1}{\hbar} \int_0^{\hbar\beta} d\tau [-\hbar g(k, \tau)] e^{iE_n \frac{\tau}{\hbar}}$

Matsubara representation $g_o(k, \tau) = \frac{1}{\hbar\beta} \sum_{iE_n} g_o(k, iE_n) e^{-iE_n \frac{\tau}{\hbar}} \quad iE_n = i \frac{\pi(2n+1)}{\beta}$

$$-G(k, iE) = (-1) \sum_{qk'g'} \frac{1}{\hbar} \int_0^{\hbar\beta} d\tau \left(-\frac{1}{\hbar} V_q\right) \int_0^{\hbar\beta} d\tau_1 \left(-\frac{1}{\hbar} V_{q'}\right) \int_0^{\hbar\beta} d\tau_2 \frac{1}{\beta} \sum_{iE_1} \sum_{iE_2} \sum_{iE_3} \sum_{iE_4} \sum_{iE_5}$$

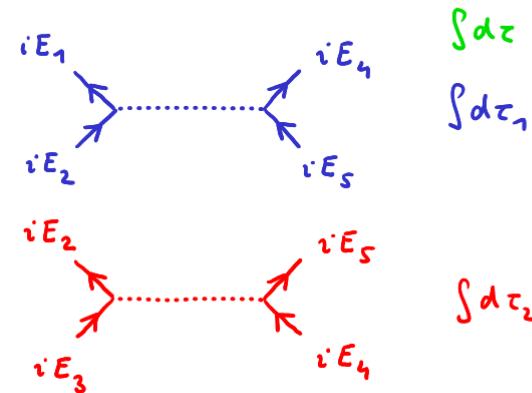
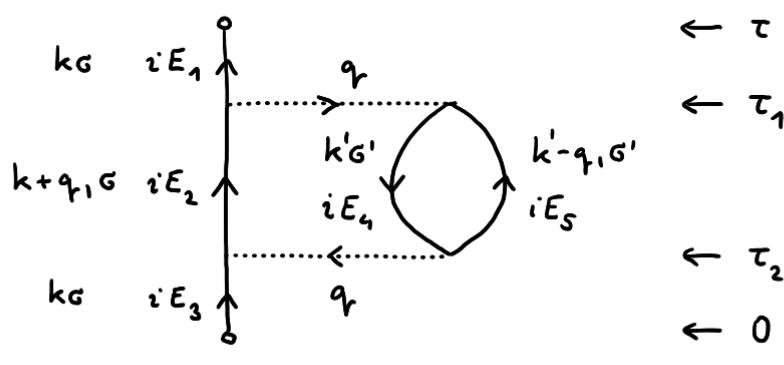
$$\left[-g_o(k, iE_1) e^{-iE_1 \frac{\tau - \tau_1}{\hbar}}\right] \left[-g_o(k+q_1, iE_2) e^{-iE_2 \frac{\tau_1 - \tau_2}{\hbar}}\right] \left[-g_o(k, iE_3) e^{-iE_3 \frac{\tau_2}{\hbar}}\right]$$

$$\left[-g_o(k', iE_4) e^{-iE_4 \frac{\tau_2 - \tau_1}{\hbar}}\right] \left[-g_o(k'-q_1, iE_5) e^{-iE_5 \frac{\tau_1}{\hbar}}\right] e^{iE_n \frac{\tau}{\hbar}}$$

- τ -integrals imply "energy conservation": $\frac{1}{\hbar} \int_0^{\hbar\beta} d\tau e^{iE \frac{\tau}{\hbar}} e^{-iE' \frac{\tau}{\hbar}} = \beta \delta_{iE, iE'}$

$$[-g_o(k, iE_1) e^{-iE_1 \frac{\tau - \tau_1}{\hbar}}] [-g_o(k+q_r, iE_2) e^{-iE_2 \frac{\tau_1 - \tau_2}{\hbar}}] [-g_o(k, iE_3) e^{-iE_3 \frac{\tau_2}{\hbar}}]$$

$$[-g_o(k', iE_4) e^{-iE_4 \frac{\tau_2 - \tau_1}{\hbar}}] [-g_o(k' - q_r, iE_5) e^{-iE_5 \frac{\tau_1 - \tau}{\hbar}}] e^{iE_n \frac{\tau}{\hbar}}$$

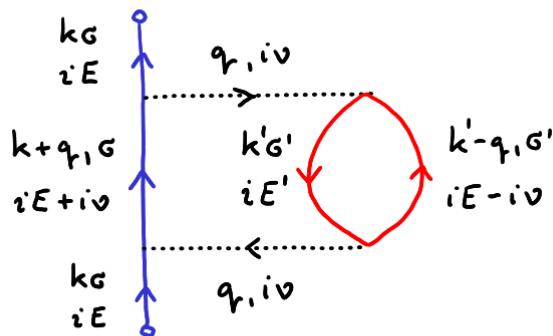


$$\int d\tau \rightarrow \delta_{iE-iE_1} \quad \int d\tau_1 \rightarrow \delta_{iE_1+iE_4-iE_2-iE_5} \quad \int d\tau_2 \rightarrow \delta_{iE_2+iE_5-iE_3-iE_4}$$

$$-g(k, iE) = (-1) \sum_{q_r k' G'} \frac{1}{\beta^2} \sum_{iE_1} \sum_{iE_2} \sum_{iE_3} \sum_{iE_4} \sum_{iE_5} (-V_{qr})^2 \delta_{iE-iE_1} \delta_{iE_1+iE_4-iE_2-iE_5} \delta_{iE_2+iE_5-iE_3-iE_4}$$

$$[-g_o(k, iE_1)] [-g_o(k+q_r, iE_2)] [-g_o(k, iE_3)] [-g_o(k', iE_4)] [-g_o(k' - q_r, iE_5)]$$

- Final G_o labels expressing the "momentum and energy flow"



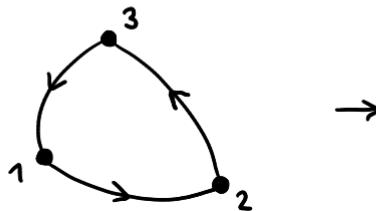
$i\nu$... bosonic Mats. frequency /energy
(difference of two fermionic)

shorthand for $i\nu_m = i \frac{2\pi m}{\beta}$ $m \in \mathbb{Z}$

summation over free momenta, q, k'
spins, and Matsubara energies $i\nu, iE'$

$$\begin{aligned}
 -G(k, iE) &= (-1) \sum_{q, k' G'} \frac{1}{\beta} \sum_{i\nu} \frac{1}{\beta} \sum_{iE'} (-V_q)^2 \times \\
 &\quad \times [-G_o(k, iE)] [-G_o(k+q, iE+i\nu)] [-G_o(k, iE)] [-G_o(k', iE')] [-G_o(k'-q, iE'-i\nu)] \\
 &= (-1) (-1)^s \sum_q (-V_q)^2 \frac{1}{\beta} \sum_{i\nu} G_o(k, iE) G_o(k+q, iE+i\nu) G_o(k, iE) \times \\
 &\quad \times \sum_{k' G'} \frac{1}{\beta} \sum_{iE'} G_o(k', iE') G_o(k'-q, iE'-i\nu) \quad \leftarrow \text{function of } q, i\nu \text{ only}
 \end{aligned}$$

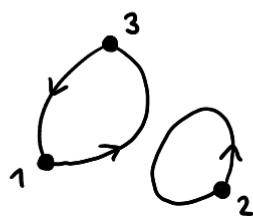
5 Sign issue - fermionic loops



$$c_1 c_3^+ c_3 c_2^+ c_2 c_1^+$$

[] [] [] [] [] []

$$-g_{13} - g_{32} - g_{21}$$



$$c_1 c_3^+ c_3 c_2^+ c_2 c_1^+$$

[] [] [] [] [] []

$$-g_{13} - g_{31} + g_{22}$$

permutation sign rule:

connect operators with threads

interchange of operators alters sign

$$\text{cc}^+ \text{cc}^+ = - \text{cc}^+ \text{cc}^+$$

→ count intersections

loop created & sign change observed $\xrightarrow{?}$ rule: each fermionic loop brings an extra -1

AGD

Attention must also be paid to the following. As already mentioned earlier, the sign attaching to each diagram depends on whether the permutation of the Fermi operators ψ is even or not. It is easily seen that a change of sign is connected with the formation of a closed loop in the diagram. The sign of the diagram is therefore determined by the factor $(-1)^F$, where F is the number of closed loops.

Rickayzen

backbone. Now it is not difficult to see that each continuous line makes its own contribution to the sign – the backbone contributes a factor $(-1)^r$ where r is the number of internal vertices on it and each closed loop contributes a factor $(-1)^{s+1}$ where s is the number of internal vertices on it. Hence, the overall factor is $(-1)^{l+2n} = (-1)^l$ where l is the number of closed loops. The overall factor for the

⑥ Dictionary

- propagators

$$\begin{array}{c} \downarrow \\ \text{k}, iE \end{array} \quad -G_0(k, iE)$$

$$\begin{array}{c} \parallel \\ \text{k}, iE \end{array} \quad -G(k, iE)$$

- interactions

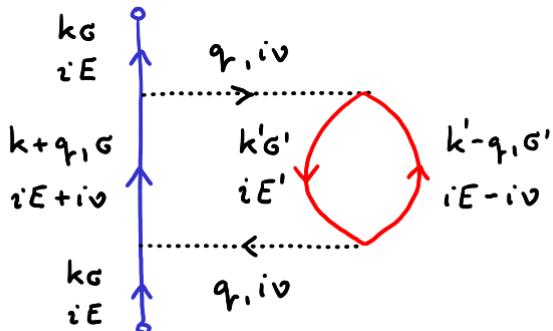
$$\begin{array}{ccc} > & \dots & < \\ q_r & & \end{array} \quad -V_{q_r}$$

- rules

1) momentum, spin, energy conservation at vertices

2) free momentum $k \rightarrow \sum_k$ free spin $\sigma \rightarrow \sum_\sigma$
 free Matsubara energy $\rightarrow \frac{1}{\beta} \sum_{iE_n}$ or $\frac{1}{\beta} \sum_{iv_m}$

3) Fermionic loops $\rightarrow (-1)^{\# \text{loops}}$



$$\begin{aligned}
 -G(k, iE) = & \dots + \\
 & \sum_{q_r} V_{q_r}^2 \frac{1}{\beta} \sum_{iv} \frac{1}{iE - \varepsilon_k} \frac{1}{iE + iv - \varepsilon_{k+q_r}} \frac{1}{iE - \varepsilon_k} \times \\
 & \times \sum_{k'g'} \frac{1}{\beta} \sum_{iE'} \frac{1}{iE' - \varepsilon_{k'}} \frac{1}{iE' + iv - \varepsilon_{k'+q_r}} \\
 & + \dots
 \end{aligned}$$