Contents

3 Diagrammatic perturbation theory

3.1 Equation of motion for G

The first item on the agenda is to introduce the Feynman rules. The idea is that, given a system described by a soluble, time independent H_0, plus an interaction term $\sim V$ considered to be small in some sense that we need to specify, we can calculate perturbative corrections to the single-particle Green's function in some formal way, e.g. the eqn. of motion method I'm about to show you. On the other hand, with this result in hand, we'll stare at the various terms (grouped according to powers of V) and notice (as Feynman did) that each term has a rather simple pictorial representation. In fact we could have written down the perturbation series without doing the formal calculation if we just had said, (aha!) the probability amplitude for a particle to get from a to b consists of the sum of the amplitudes for it to make it from a to b in all possible ways. It's relatively easy to imagine pictures of all possible ways, and with a few simple rules to take care of multiplicities, minus signs, etc. we can do the calculation much more easily.

3.1.1 Impurity problem

I'm going to start with a simple example which doesn't really involve particles colliding with each other, but rather with a set of randomly distributed, localized one-body potentials. If the particles are fermions, this is a pretty good model of impurities in a metal. If they are bosons, one could think of ^{4}He atoms adsorbed on a rough surface, (??? other physical systems).

First let's consider one impurity only, described by a potential $U(\mathbf{r}, \tau)$ (we will do everything in finite temperature/ imaginary time formalism from here on out). The equation of motion for the Green's function

$G(\mathbf{r}_1, \tau_1; \mathbf{r}_2, \tau_2)$ is[1]

$$\boxed{\left[\partial_{\tau_1} + h_0(\mathbf{r}) + U(\mathbf{r}, \tau_1)\right] G(\mathbf{r}_1, \tau_1; \mathbf{r}_2, \tau_2) = -\delta(\mathbf{r}_1 - \mathbf{r}_2)\delta(\tau_1 - \tau_2),} \quad (1)$$

where h_0 is the unperturbed 1st-quantized hamiltonian density, $H_0 = \int d^3 r h_0(\mathbf{r})$ (usually $h_0 = -\nabla^2/(2m)$). Note (1) is the mathematical and semantic connection between the "Green's function" as quantum probability amplitude we have been studying, and the classical "Green's function" in, e.g. electromagnetic theory, which is the inverse of a differential operator.[2]

The notation is going to get pretty hairy, so we can make our lives easier by going to a kind of 4-vector notation, e.g. $1 = \mathbf{r}_1, \tau_1$, $2 = \mathbf{r}_2, \tau_2$, etc. Separate $\mathbf{r}$ and τ only when necessary, e.g. (1) is just

$$\boxed{[\partial_{\tau_1} + h(1)]G(1;2) = -\delta(1-2)}, \quad (2)$$

where $h = h_0 + U$. Of course we are supposed to know the solution G_0 in the absence of U:

$$[\partial_{\tau_1} + h_0(1)]G_0(1;2) = -\delta(1-2), \quad (3)$$

And don't forget we are looking solutions to this differential equation subject to the boundary condition that the Green's function have the right analytic form (periodicity properties in time):

$$G(\underbrace{0}_{\mathbf{r}_1, \tau_1 = 0};2) = \pm G(\beta;2) \qquad \tau_2 > 0 \quad (4)$$

Now a formal integration can be performed, giving

$$G(1;2) = G_0(1;2) + \int_0^\beta d3\; G_0(1;3)U(3)G(3;2), \quad (5)$$

where $\int d3 \equiv \int \tau_3 \int d^3 r_3$. Plug it in and see that it works![3] Now we can

[1] give proof here?

[2] George Green (1793-1841) didn't know much about quantum mechanics.

[3] You'll need to be courageous about pulling differential operators through integral signs, e.g

$$\begin{aligned}[\partial_{\tau_1} + h_0(1)] \int_0^\beta d3 G_0(1;3)U(3)G(3;2) &= \int_0^\beta d3\left([\partial_{\tau_1} + h_0(1)]G_0(1;3)\right) \\ &= \int_0^\beta d3(-\delta(1-3))U(3)G(3;2) = -U(1)G(1;2)\end{aligned}$$

iterate formal solution,

$$
\begin{aligned}
G(1;2) &= G_0(1;2) + \int_0^\beta d3 G_0(1;3)U(3)G_0(3;2) + & (6)\\
&+ \int_0^\beta d3 \int_0^\beta d3' G_0(1;3)U(3)G_0(3;3')U(3')G_0(3';2) + \ldots & (7)
\end{aligned}
$$

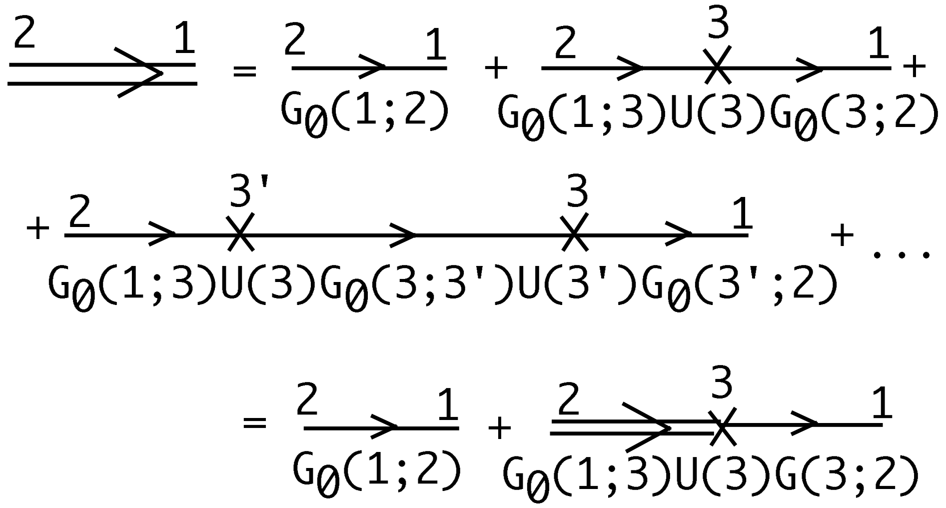
Note products have *matrix* structure, with $(U(a,b) \propto \delta_{ab})$. So could write schematically

$$G = G_0 + G_0UG_0 + G_0UG_0UG_0 + \ldots \tag{8}$$

if we remember to integrate over the internal time and space indices.

⋆Diagrams

Represent terms in (8) by diagrams:



Physics: probability amplitude that the particle propagates from 2 to 1 is sum of amplitude that it propagates without scattering from 2 to 1, plus amplitude it scatters once (summed over all positions and times where this can happen), plus amplitude where it scatters twice, etc.

Remarks:

- Double line represents G, single line G_0.
- Note convention of argument order in diagrams and Green's functions: $G(1;2) = -\langle \mathcal{T}_\tau \hat{\psi}(1)\hat{\psi}(2)\rangle$ is amplitude for particle to be created at 2 and then propagate to 1, when it is destroyed, as reflected in diagrams.

- Note in last step in figure, the series was resummed to represent the integral equation (5) with only two terms; note the occurence of $G(3;2)$ instead of $G_0(3;2)$ in second term.

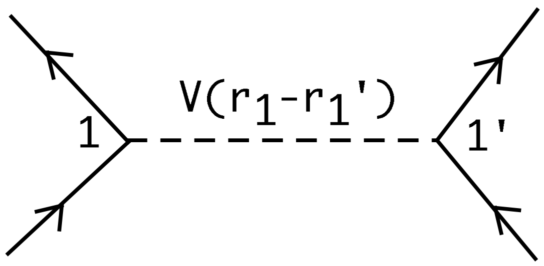
- If $\tau_2 > \tau_1$, process represents *hole* propagation. Term in G is $\langle\hat{\psi}^\dagger(2)\hat{\psi}(1)\rangle\theta(\tau_2-\tau_1)$: hole created at 1, destroyed at later time 2. Or: particle destroyed at 1 before being created at 2 $\rightarrow$ particle propagating backwards in time.

3.1.2 Interacting systems: qualitative

If there is a two-body interaction $V(1,2)$ present, i.e. the Hamiltonian is

$$\hat{H} = \hat{H}_0 + \frac{1}{2}\int d^3r d^3r' \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r}')V(\mathbf{r},\mathbf{r}')\hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r}), \tag{9}$$

we might expect to construct a similar series diagramatically.[4] The interaction looks like this:



You see there is both a creation and a destruction operator in (9) for both $\mathbf{r}_1$ and $\mathbf{r}'_1$; this is to be thought of as a scattering process of the particle on

[4] The equation of motion method for G is not as straightforward. It looks like

$$\begin{aligned}[\partial_{\tau_1} + h_0(\mathbf{r}_1) + U(\mathbf{r}_1,\tau_1)]G(1;2)&\\ \mp\int d1' v(1-1')G(1;\mathbf{r}_2,\tau_1;1';\mathbf{r}_2,\tau_1^+)&\\ = -\delta(\mathbf{r}_1-\mathbf{r}_2)\delta(\tau_1-\tau_2)&\end{aligned} \tag{10}$$

where I've introduced the *2-particle Green's function*

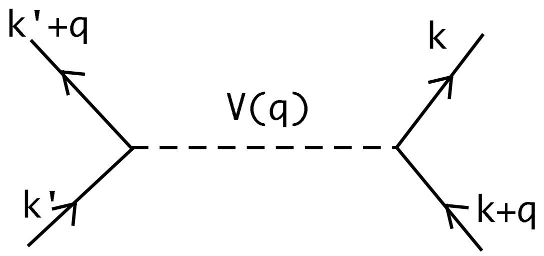
$$G(1;2;3;4) \equiv \langle \mathcal{T}_\tau \left[\hat{\psi}(\mathbf{r}_1,\tau_1)\hat{\psi}(r_2,\tau_2)\hat{\psi}^\dagger(\mathbf{r}_3,\tau_3)\hat{\psi}^\dagger(\mathbf{r}_4,\tau_4)\right]\rangle \tag{11}$$

So to find the τ-dependence of the 1-particle Green's function you need to find the τ-dependence of the 2-particle Green's function, and so on. See sec. xxx.

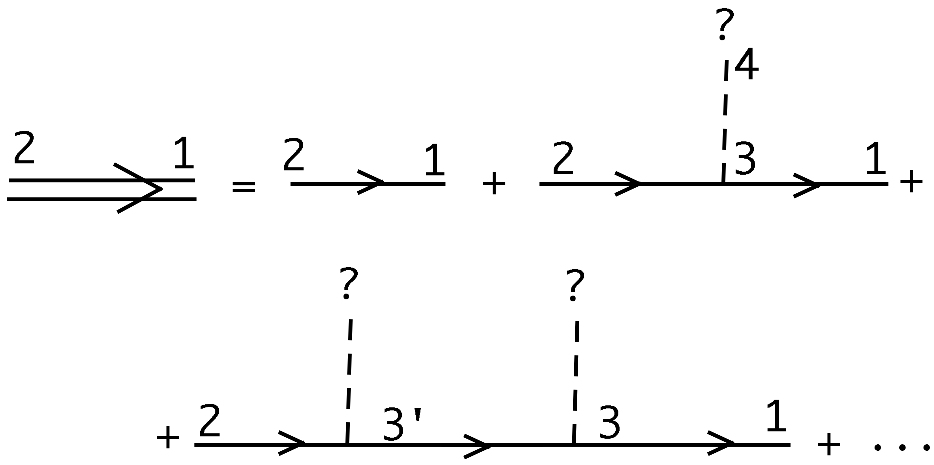
the left by the particle on the right, with $V(1,1')$ the scattering potential between them.[5] In fact, in Fourier transform language,

$$\hat{V} = \frac{1}{2}\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} a^\dagger_{\mathbf{k}} a^\dagger_{\mathbf{k}'+\mathbf{q}} V(\mathbf{q}) a_{\mathbf{k}'} a_{\mathbf{k}+\mathbf{q}} \tag{12}$$

which then looks like this:



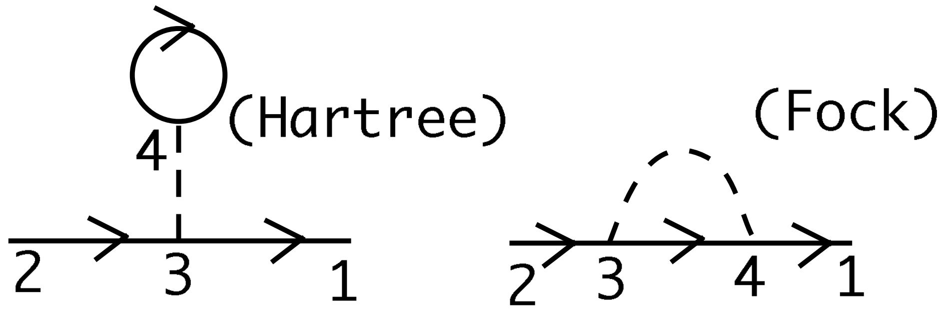
How can we draw diagrams representing the propagation of a single particle, occasionally scattering off its compatriots? Look at the following picture:



As before, our intuition might be, the particle propagates along, either doesn't scatter at all, or perhaps scatters once, as in 2nd term on rhs, etc. But this time it scatters not with a fixed impurity, but with another particle. Where is the other particle in the picture? Well, it has to be represented by another particle propagating, i.e. by a separate Green's function line. I therefore can't leave the interaction lines dangling, but

[5] In relativistic field theory, V is frequently viewed as having a particle-like nature itself, it propagates at the speed of light, and one speaks of the interaction being "mediated by the exchange of a particle". Here in the nonrelativistic theory we can replace the "photon" by a static potential because the speed of light is too fast for us.

have to attach a propagator line somehow; these have to close on themselves somehow, or they will remain dangling themselves. Two obvious possibilities are



which we will encounter again.

3.2 Derivation of perturbation series

3.2.1 S-matrix

Recall relation between Heisenberg and interaction pictures:

$$\hat{\mathcal{O}}_I(\tau) = e^{\hat{K}_0\tau}\hat{\mathcal{O}}_S e^{-\hat{K}_0\tau} \tag{13}$$

$$\hat{\mathcal{O}}_H(\tau) = e^{\hat{K}\tau}\hat{\mathcal{O}}_S e^{-\hat{K}\tau} \tag{14}$$

$$\begin{aligned}\Rightarrow \hat{\mathcal{O}}_H(\tau) &= e^{\hat{K}\tau}e^{-\hat{K}_0\tau}\hat{\mathcal{O}}_I(\tau)e^{\hat{K}_0\tau}e^{-\hat{K}\tau} \\ &= \hat{S}(0,\tau)\hat{\mathcal{O}}_I(\tau)\hat{S}(\tau,0)\end{aligned} \tag{15}$$

where

$$\hat{S}(\tau_1,\tau_2) = e^{\hat{K}_0\tau_1}e^{-\hat{K}(\tau_1-\tau_2)}e^{-\hat{K}_0\tau_2} \tag{16}$$

Remarks:

- $\hat{S}$ *not* unitary for τ real.
- group property $\hat{S}(\tau_1,\tau_2)\hat{S}(\tau_2,\tau_3) = S(\tau_1,\tau_3)$
- boundary condition $\hat{S}(\tau_1,\tau_1) = 1$

• eqn. of motion for $\hat{S}$:

$$\begin{aligned}\partial_\tau \hat{S}(\tau,\tau') &= e^{\hat{K}_0\tau}(\hat{K}_0 - \hat{K})e^{-\hat{K}(\tau-\tau')}e^{-\hat{K}_0\tau'} \\ &= e^{\hat{K}_0\tau}(\hat{K}_0 - \hat{K})e^{-\hat{K}_0\tau}\hat{S}(\tau,\tau')\end{aligned}$$

$$\Rightarrow \qquad \boxed{\partial_\tau \hat{S}(\tau,\tau') = -\hat{V}_I(\tau)\hat{S}(\tau,\tau')} \tag{17}$$

where

$$\hat{K} = \hat{H}_0 - \mu\hat{N} + \hat{V} \quad ; \quad \hat{V}_I(\tau) = e^{\hat{K}_0\tau}\hat{V}e^{-\hat{K}_0\tau} \tag{18}$$

• Formal solution for S-matrix: Integrate eqn. of motion from τ_0 to τ:[6]

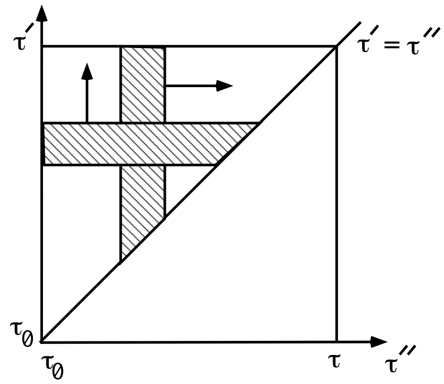
$$\boxed{\hat{S}(\tau,\tau_0) - \hat{S}(\tau_0,\tau_0) = \int_{\tau_0}^{\tau} d\tau'\ \hat{V}_I(\tau')\hat{S}(\tau',\tau_0)} \tag{19}$$

• Iterate:

$$\boxed{\hat{S}(\tau,\tau_0) = \sum_{n=0}^{\infty}(-1)^n\frac{1}{n!}\int_{\tau_0}^{\tau} d\tau_1 \cdots \int_{\tau_0}^{\tau} d\tau_n \mathcal{T}_\tau\left[\hat{V}_I(\tau_1)\cdots\hat{V}_I(\tau_n)\right]} \tag{20}$$

⋆ Q: Where does time-ordering symbol come from? Consider third term in iteration of (19):

$$\begin{aligned}&(-1)^2\int_{\tau_0}^{\tau} d\tau' \int_{\tau_0}^{\tau'} d\tau''\hat{V}_I(\tau')\hat{V}_I(\tau'') \\ = \ &(-1)^2\frac{1}{2}\left[\int_{\tau_0}^{\tau} d\tau' \int_{\tau_0}^{\tau'} d\tau''\hat{V}_I(\tau')\underbrace{\hat{V}_I(\tau'') + \int_{\tau_0}^{\tau} d\tau'' \int_{\tau''}^{\tau} d\tau'\hat{V}_I(\tau')}_{\text{same area}}\hat{V}_I(\tau'')\right]\end{aligned}$$



Now change dummy variables in 2nd term $\tau' \leftrightarrow \tau''$, then combine:

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[6]Mathematical note: integral eqn. is of Volterra form. If $\hat{S}$ were c-number function, iterative soln. almost always converges (broad range of well-defined conditions). Convergence not necessarily guaranteed for $\hat{S}$ operator, nevertheless try solution of this type, respecting *order* of operators

$$= (-1)^2 \frac{1}{2} \int_{\tau_0}^{\tau} d\tau' \left\{ \int_{\tau_0}^{\tau'} d\tau'' \hat{V}_I(\tau')\hat{V}_I(\tau'') + \int_{\tau'}^{\tau} d\tau'' \hat{V}_I(\tau'')\hat{V}_I(\tau') \right\}$$
$$= (-1)^2 \frac{1}{2} \int_{\tau_0}^{\tau} d\tau' \int_{\tau_0}^{\tau} d\tau'' \left\{ \hat{V}_I(\tau')\hat{V}_I(\tau'')\theta(\tau'-\tau'') + \hat{V}_I(\tau'')\hat{V}_I(\tau')\theta(\tau''-\tau') \right\}$$
$$= (-1)^2 \frac{1}{2} \int_{\tau_0}^{\tau} d\tau' \int_{\tau_0}^{\tau} d\tau'' \; \mathcal{T}_\tau[\hat{V}_I(\tau')\hat{V}_I(\tau'')]$$

⋆ And now we understand (sort of) why time-ordered function is useful for perturbation theory: time-ordered products of interactions occur naturally in the S-matrix, which can now be written[7]

$$\boxed{S(\tau,\tau_0) = \mathcal{T}_\tau \exp\left[-\int_{\tau_0}^{\tau} d\tau_1 \hat{V}_I(\tau_1) \right]} \tag{21}$$

3.2.2 Perturbation series for G

- Green's function in interaction representation for

  a) $\underline{\tau > \tau'}$:

$$G(\mathbf{r},\tau;\mathbf{r}',\tau') = -\frac{1}{\underbrace{\mathrm{Tr} e^{-\beta\hat{K}}}_{\equiv Z}} \mathrm{Tr}\left[e^{-\beta\hat{K}} \hat{\psi}_H(\mathbf{r},\tau)\hat{\psi}_H^\dagger(\mathbf{r}',\tau') \right]$$
$$= -\frac{1}{Z}\mathrm{Tr}\left[e^{-\beta\hat{K}_0} S(\beta,0) \left(S(0,\tau)\hat{\psi}_I(\mathbf{r},\tau)S(\tau,0) \right) \left(S(0,\tau')\hat{\psi}_I^\dagger(\mathbf{r}',\tau')S(\tau',0) \right) \right]$$
$$= -\frac{1}{Z}\mathrm{Tr}\left[e^{-\beta\hat{K}_0} S(\beta,\tau)\hat{\psi}_I(\mathbf{r},\tau)S(\tau,\tau')\hat{\psi}_I^\dagger(\mathbf{r}',\tau')S(\tau',0) \right] \tag{22}$$

  and similarly, find

  b) $\underline{\tau < \tau'}$:

$$G(\mathbf{r},\tau;\mathbf{r}',\tau') = \mp\frac{1}{Z}\mathrm{Tr}\left[e^{-\beta\hat{K}_0} S(\beta,\tau')\hat{\psi}_I^\dagger(\mathbf{r}',\tau')S(\tau',\tau)\hat{\psi}_I(\mathbf{r},\tau)S(\tau,0) \right] \tag{23}$$

[7] Expand the exponential carefully and you'll get Eq. (20).

- Expand S-matrix and collect terms:

$$\boxed{G(\mathbf{r},\tau;\mathbf{r}',\tau') = \frac{-\mathrm{Tr}\left\{e^{-\beta\hat{K}_0}\sum_{n=0}^{\infty}(-1)^n\frac{1}{n!}\int_0^\beta d\tau_1\cdots\int_0^\beta d\tau_n\mathcal{T}_\tau\left[\hat{V}_I(\tau_1)\cdots\hat{V}_I(\tau_n)\hat{\psi}(\mathbf{r},\tau)\hat{\psi}^\dagger(\mathbf{r}',\tau')\right]\right\}}{-\mathrm{Tr}\left\{e^{-\beta\hat{K}_0}\sum_{n=0}^{\infty}(-1)^n\frac{1}{n!}\int_0^\beta d\tau_1\cdots\int_0^\beta d\tau_n\mathcal{T}_\tau\left[\hat{V}_I(\tau_1)\cdots\hat{V}_I(\tau_n)\right]\right\}}} \tag{24}$$

Now this looks pretty horrible,[8] but there is one enormous simplification: notice that expectation values of the products $\hat{V}_I\hat{V}_I...\hat{V}_I\hat{\psi}\hat{\psi}^\dagger$ are taken in the *noninteracting ensemble*, $\mathrm{Tr}\{e^{-\beta\hat{K}_0}\ldots\}$. So if we can figure out how to decompose averages of long products of many operators into products of averages of *pairs* of operators, we can simply use the noninteracting Green's function G_0. This is the essence of Wick's theorem.

3.2.3 Wick's theorem

- Statement of Wick's theorem

Define *contraction*:

given two operators $\hat{A}$ and $\hat{B}$, the *contraction* is

$$\underbrace{\hat{A}\hat{B}} = \mathrm{Tr}(\rho_0\mathcal{T}_\tau(\hat{A}\hat{B}) \equiv \langle\hat{A}\hat{B}\rangle_0 \tag{25}$$

Then:

$$\boxed{\langle\mathcal{T}_\tau\hat{A}\hat{B}\cdots\hat{F}\rangle_0 = \langle\mathcal{T}_\tau\left\{\underbrace{\hat{A}\hat{B}}\hat{C}\cdots\hat{F} + \underbrace{\hat{A}\hat{B}\hat{C}}\cdots\hat{F}+\cdots\right\}\rangle,} \tag{26}$$

[8]It is perhaps not obvious how to arrive at the result(24), given that (22) contains the factors $\hat{S}(\beta,\tau)$, $\hat{S}(\tau,\tau')$, etc., each of which has its own time ordering, but (24) contains only terms like $V_I(\tau_1)\cdots V_I(\tau_n)\hat{\psi}(\tau)\hat{\psi}^\dagger(\tau')$. Write out the defs. of $\hat{S}$ in (22):

$$\begin{aligned} G(\mathbf{r},\tau;\mathbf{r}',\tau') &= -\frac{1}{Z}\mathrm{Tr}\left[e^{-\beta\hat{K}_0}S(\beta,\tau)\hat{\psi}_I(\mathbf{r},\tau)S(\tau,\tau')\hat{\psi}_I^\dagger(\mathbf{r}',\tau')S(\tau',0)\right] \\ &= -\frac{1}{Z}\mathrm{Tr}\left[e^{-\beta\hat{K}_0}\mathcal{T}_\tau\exp\left\{-\int_\tau^\beta\hat{V}_I(\tau_1)d\tau_1\right\}\hat{\psi}_I(\mathbf{r},\tau)\mathcal{T}_\tau\exp\left\{-\int_{\tau'}^\tau\hat{V}_I(\tau_1)d\tau_1\right\}\hat{\psi}_I^\dagger(\mathbf{r}',\tau')\mathcal{T}_\tau\exp\left\{-\int_0^{\tau'}\hat{V}_I(\tau_1)d\tau_1\right\}\right] \end{aligned}$$

and then notice that everything consists of products of interaction operators in the "proper" time ordering, even for all the intermediate times in the integrations. This means that all the time-ordered exponentials $\hat{S}$ may be commuted with the $\hat{\psi}$ operators, provided they are kept inside one overall time-ordering operator. But then the arguments of the exponentials may be added, giving integrals over the full time range 0 to β, yielding (24) i.e. *take all possible full contractions of all pairs of operators and add them.*[9] Note that in the case of fermion operators there are signs involving commutation of operators past each other, e.g.

$$\hat{A}\hat{C}\hat{B}\cdots\hat{F} = \pm\hat{A}\hat{B}\hat{C}\cdots\hat{F} \tag{27}$$

Example:[10]

$$\langle T_\tau ABCD\rangle = A\;B\;C\;D + A\;B\;C\;D + A\;B\;C\;D$$

$$= \underbracket{A\;B}\;\underbracket{C\;D} - \underbracket{A\;C}\;\underbracket{B\;D} + \underbracket{A\;D}\;\underbracket{B\;C}$$

- Proof of Wick's theorem $(T > 0)$ for $\tau_a > \tau_b > \cdots > \tau_f$[11]

  We want to evaluate products like $\langle\hat{A}\hat{B}\cdots\hat{F}\rangle_0$, where $\hat{A}$, etc. are interaction picture operators like $\hat{\psi}_I(\tau)$ or $\hat{\psi}_I^\dagger(\tau)$.

  – First, express in terms of creation & annihilation ops. a_i and $a_i^\dagger$ for single-particle states i of H_0, e.g.

  $$\hat{A} = \sum_i \Phi_i(\mathbf{r},\tau)\alpha_i = \begin{cases} \Sigma_i\,\phi_i^0(\mathbf{r})e^{-\xi_i\tau}a_i & \hat{A} = \hat{\psi} \\ \Sigma_i\,\phi_i^{0*}(\mathbf{r})e^{\xi_i\tau}a_i^\dagger & \hat{A} = \hat{\psi}^\dagger \end{cases}$$

  (recall τ-dependence of operators is trivial in interaction picture!) Then

  $$\langle\hat{A}\hat{B}\cdots\hat{F}\rangle_0 = \sum_{a,b,c\ldots,f}\Phi_a\Phi_b\cdots\Phi_f\;\mathrm{Tr}\left(\hat{\rho}_0\alpha_a\alpha_b\cdots\alpha_f\right) \tag{28}$$

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[9] not only all contractions of $\hat{A}$ with other operators, which would give a c-number times a product of N-2 operators, but all other contractions of pairs as well. (This is difficult to state clearly in words or symbols, but it is fairly clear after one has done a couple of examples!)

[10] Not all these terms may occur. For example,

$$\begin{aligned}\langle\mathcal{T}_\tau\hat{\psi}(\tau_A)\hat{\psi}^\dagger(\tau_B)\hat{\psi}(\tau_C)\hat{\psi}^\dagger(\tau_D)\rangle_0 &= \langle\mathcal{T}_\tau\hat{\psi}(\tau_A)\hat{\psi}^\dagger(\tau_B)\rangle_0\langle\mathcal{T}_\tau\hat{\psi}(\tau_C)\hat{\psi}^\dagger(\tau_D)\rangle_0 \\ &\quad+\langle\mathcal{T}_\tau\hat{\psi}(\tau_A)\hat{\psi}^\dagger(\tau_D)\rangle_0\langle\mathcal{T}_\tau\hat{\psi}^\dagger(\tau_B)\hat{\psi}(\tau_C)\rangle_0 \\ &\equiv G_0(\tau_A-\tau_B)G_0(\tau_B-\tau_C)\pm G_0(\tau_A-\tau_D)G_0(\tau_C-\tau_B).\end{aligned}$$

The BD;AC contraction doesn't occur because particle number is not conserved.

[11] Proving for this time ordering is sufficient since definition of contractions ensures that - signs accounted for, & all possible contractions occur

where $\alpha = a$ or $a^\dagger$. Note there must be an equal number of a's and $a^\dagger$'s in the usual case with fixed particle number.

– Consider $\mathrm{Tr}(\hat{\rho}_0\alpha_a\cdots\alpha_f)$: commute α_a succesively to right:

$$\begin{aligned}
\mathrm{Tr}(\hat{\rho}_0\alpha_a\alpha_b\cdots\alpha_f) &= \mathrm{Tr}(\hat{\rho}_0[\alpha_a,\alpha_b]_\mp\alpha_c\cdots\alpha_f) \pm \mathrm{Tr}(\hat{\rho}_0\alpha_b[\alpha_a,\alpha_c]_\mp\alpha_d\cdots\alpha_f) \\
&\quad \underbrace{+\cdots+}_{\text{alternate + and }\pm} \quad \mathrm{Tr}(\hat{\rho}_0\alpha_b\alpha_c\cdots[\alpha_a,\alpha_f]_\mp) \pm \mathrm{Tr}(\hat{\rho}_0\alpha_b\alpha_c\cdots\alpha_f\alpha_a)
\end{aligned} \tag{29}$$

– Note $e^{\beta\hat{K}_0}\alpha_a e^{-\beta\hat{K}_0} = \alpha_a e^{\lambda_a\beta\xi_a}$, where $\lambda_a = \pm1$ for $\left\{\begin{array}{c}\text{creation } a^\dagger \\ \text{annihilation } a\end{array}\right.$.

Therefore $\alpha_a\hat{\rho}_0 = \hat{\rho}_0\alpha_a e^{\lambda_a\beta\xi_a}$

– Note last term in Eq. (29)

$$\begin{aligned}
\pm\mathrm{Tr}(\hat{\rho}_0\alpha_b\alpha_c\cdots\alpha_f\alpha_a) &= \pm\mathrm{Tr}(\alpha_a\hat{\rho}_0\alpha_b\alpha_c\cdots\alpha_f) \\
&= \pm e^{\lambda_a\beta\xi_a}\mathrm{Tr}(\hat{\rho}_0\alpha_a\alpha_b\alpha_c\cdots\alpha_f)
\end{aligned}$$

Bring to lhs of (29); divide by $1 \mp e^{\lambda_a\beta\xi_a}$:

$$\begin{aligned}
\mathrm{Tr}(\hat{\rho}_0\alpha_a\alpha_b\cdots\alpha_f) &= \frac{[\alpha_a,\alpha_b]_\mp}{1\mp e^{\lambda_a\beta\xi_a}}\mathrm{Tr}(\hat{\rho}_0\alpha_c\cdots\alpha_f) \pm \frac{[\alpha_a,\alpha_c]_\mp}{1\mp e^{\lambda_a\beta\xi_a}}\mathrm{Tr}(\hat{\rho}_0\alpha_b\alpha_d\cdots\alpha_f) \\
&\quad \underbrace{+\cdots+}_{\text{alternate + and }\pm} \quad + \frac{[\alpha_a,\alpha_f]_\mp}{1\mp e^{\lambda_a\beta\xi_a}}\mathrm{Tr}(\hat{\rho}_0\alpha_b\alpha_c\cdots\alpha_e)
\end{aligned}$$

– Define contraction:

$$\underbrace{\alpha_a\alpha_b} \equiv \frac{[\alpha_a,\alpha_b]_\mp}{1\mp e^{\lambda_a\beta\xi_a}} \tag{30}$$

For example,

$$\underbrace{a_i^\dagger a_i} = \frac{[a_i^\dagger,a_i]_\mp}{1\mp e^{\beta\xi_i}} = \frac{\pm1}{1\mp e^{\beta\xi_i}} = \begin{array}{c} b(\xi_i) \\ f(\xi_i)\end{array} \tag{31}$$

and

$$\underbrace{a_i a_i^\dagger} = \frac{[a_i,a_i^\dagger]_\mp}{1\mp e^{-\beta\xi_i}} = \frac{1}{1\mp e^{-\beta\xi_i}} = \begin{array}{c} 1+b(\xi_i) \\ 1-f(\xi_i)\end{array} \tag{32}$$

And all other contractions are zero, from fundamental commutation relations! Reminder: $\underbracket{\alpha_a\alpha_b} = \langle\alpha_a\alpha_b\rangle_0 = \langle\mathcal{T}_\tau\alpha_a\alpha_b\rangle_0$ since $\tau_a > \tau_b$ by assumption.

– Left with

$$\begin{aligned}\mathrm{Tr}(\hat{\rho}_0\alpha_a\alpha_b\cdots\alpha_f) &= \underbracket{\alpha_a\alpha_b}\mathrm{Tr}(\hat{\rho}_0\alpha_c\cdots\alpha_f) \pm \underbracket{\alpha_a\alpha_c}\mathrm{Tr}(\hat{\rho}_0\alpha_b\alpha_d\cdots\alpha_f) \\ &\quad \underbrace{+\cdots+}_{\text{alternate + and }\pm} \quad +\underbracket{\alpha_a\alpha_f}\mathrm{Tr}(\hat{\rho}_0\alpha_b\alpha_c\cdots\alpha_e).\end{aligned}$$

The remaining traces can be expanded in exactly the same way; furthermore since the contractions are c-numbers, they can be pulled in and out of the traces; if they are put back in the original ordering, the - signs go away according to the definition (27).

$$\begin{aligned}\mathrm{Tr}(\hat{\rho}_0\alpha_a\alpha_b\cdots\alpha_f) &= \mathrm{Tr}(\hat{\rho}_0\underbracket{\alpha_a\alpha_b}\alpha_c\cdots\alpha_f) + \mathrm{Tr}(\hat{\rho}_0\underbracket{\alpha_a\alpha_b\alpha_c}\alpha_d\cdots\alpha_f) \\ &\quad +\cdots+\mathrm{Tr}(\hat{\rho}_0\underbracket{\alpha_a\alpha_b\alpha_c\cdots\alpha_e\alpha_f}).\end{aligned}$$

– Sums over i can be reintroduced as in Eq. (28), giving

$$\boxed{\langle\hat{A}\hat{B}\cdots\hat{F}\rangle_0 = \text{sum of all possible products of pairs of contractions}} \tag{33}$$

- Remarks:

1. We assumed only evolution of I-picture operators according to soluble $\hat{H}_0$.
2. Wick's theorem in its original form is an operator identity: it relates a time-ordered product to a sum of *normal-ordered* products (put annihilation part of field operators to right). The generalized theorem I discuss here holds at nonzero temperatures, but only for the ensemble average (Matsubara 1955).

3.2.4 Diagrams for interacting systems

- Return to perturbation series for G and apply Wick's theorem:

$$\boxed{G(\mathbf{r},\tau;\mathbf{r}',\tau')=\frac{-\mathrm{Tr}\left\{e^{-\beta\hat{K}_0}\sum_{n=0}^{\infty}(-1)^n\frac{1}{n!}\int_0^\beta d\tau_1\cdots\int_0^\beta d\tau_n\mathcal{T}_\tau\left[\hat{V}_I(\tau_1)\cdots\hat{V}_I(\tau_n)\hat{\psi}(\mathbf{r},\tau)\hat{\psi}^\dagger(\mathbf{r}',\tau')\right]\right\}}{-\mathrm{Tr}\left\{e^{-\beta\hat{K}_0}\sum_{n=0}^{\infty}(-1)^n\frac{1}{n!}\int_0^\beta d\tau_1\cdots\int_0^\beta d\tau_n\mathcal{T}_\tau\left[\hat{V}_I(\tau_1)\cdots\hat{V}_I(\tau_n)\right]\right\}}}$$

And recall also

$$\hat{V}_I(\tau_1)=e^{\tau_1\hat{K}_0}\left[\frac{1}{2}\int d^3rd^3r'\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r}')V(\mathbf{r}-\mathbf{r}')\psi^\dagger(\mathbf{r}')\psi^\dagger(\mathbf{r})\right]e^{-\tau_1\hat{K}_0} \qquad (34)$$

- Define $v(x-x')\equiv V(\mathbf{r}-\mathbf{r}')\delta(t-t')$, $\hat{\psi}(x)\equiv e^{\tau_1\hat{K}_0}\hat{\psi}(\mathbf{r})e^{-\tau_1\hat{K}_0}$, so e.g.

$$\int_0^\beta d\tau_1\hat{V}_I(\tau_1)=\frac{1}{2}\int d^4xd^4x'\hat{\psi}^\dagger(x)\hat{\psi}^\dagger(x')v(x-x')\hat{\psi}(x')\hat{\psi}(x)$$

- Examine numerator of G (call it $\overline{G}$) term by term:

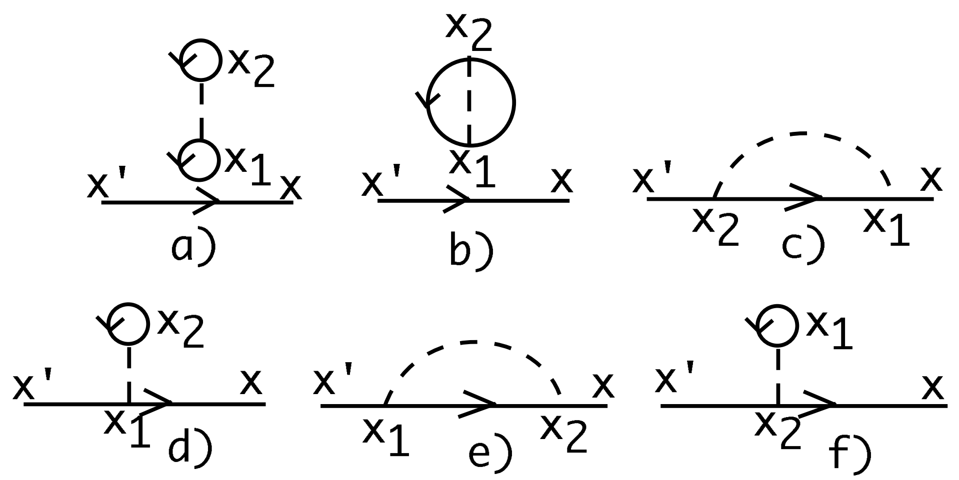
$$\overline{G}=\overline{G}_0+\overline{G}_1+\overline{G}_2+\ldots \qquad (35)$$

Example (1st order):

$$\begin{aligned}
\overline{G}_1(x,x') &= \frac{1}{2}\mathrm{Tr}\left(e^{-\beta\hat{K}_0}\mathcal{T}_\tau\int d^4x_1d^4x_2\ v(x_1-x_2)\hat{\psi}^\dagger(x_1)\hat{\psi}^\dagger(x_2)\hat{\psi}(x_2)\hat{\psi}(x_1)\hat{\psi}(x)\hat{\psi}(x')\right)\\
&= \frac{1}{2}\int d^4x_1d^4x_2\ v(x_1-x_2)\langle\mathcal{T}_\tau\hat{\psi}^\dagger(x_1)\hat{\psi}^\dagger(x_2)\hat{\psi}(x_2)\hat{\psi}(x_1)\hat{\psi}(x)\hat{\psi}(x')\rangle_0\\
(Wick) &= \frac{1}{2}\int d^4x_1d^4x_2\ v(x_1-x_2)\times\\
&\quad Z_0\left[G_0(x,x')\left(\underbrace{G_0(x_2,x_2)G_0(x_1,x_1))}_{a}-\underbrace{G_0(x_1,x_2)G_0(x_2,x_1)}_{b}\right)\right.\\
&\quad +G_0(x,x_1)\left(\underbrace{G_0(x_2,x')G_0(x_1,x_2)}_{c}-\underbrace{G_0(x_2,x_2)G_0(x_1,x')}_{d}\right)\\
&\quad \left.+G_0(x,x_2)\left(\underbrace{G_0(x_2,x_1)G_0(x_1,x')}_{e}-\underbrace{G_0(x_2,x')G_0(x_1,x_1)}_{f}\right)\right],
\end{aligned} \qquad (36)$$

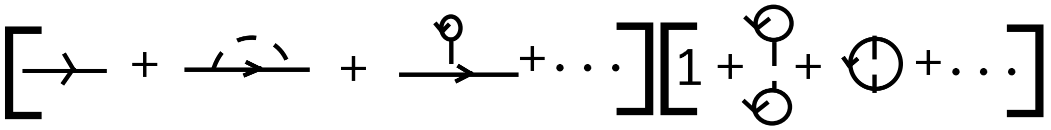
and Z_0 is zeroth-order term in partition fctn., see below.

- Feynman diagrams for first-order processes (numerator only!):



- Numerator *factorizes.*

Compare a few more terms and you see numerator can be written



⋆<u>Remarks</u>:

 – There are two diagrams of each type in 1st order; cancel with factor of 1/2 from V_I.
 – Second factor (the sum of *disconnected* diagrams) is nothing more than the partition function:

$$\text{denominator} = Z \;=\; Z_0 + Z_1 + Z_2 + \dots$$

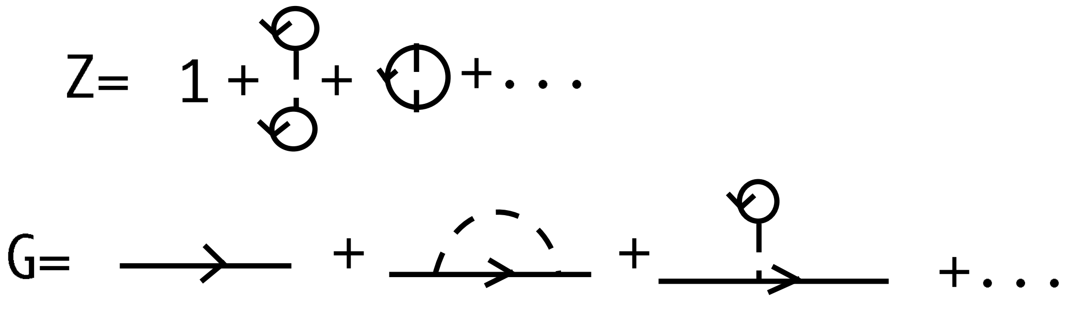
e.g., 1st order

$$\begin{aligned} Z_1 &= \frac{1}{2}\int d^4x_1 d^4x_2\; v(x_1 - x_2)\langle \mathcal{T}_\tau \hat{\psi}^\dagger(x_1)\hat{\psi}^\dagger(x_2)\hat{\psi}(x_2)\hat{\psi}(x_1)\rangle_0 \\ &= \frac{1}{2}\int d^4x_1 d^4x_2\; v(x_1 - x_2) Z_0 \left[G_0(x_2, x_2)G_0(x_1, x_1) - G_0(x_1, x_2)G_0(x_2, x_1)\right] \end{aligned}$$

which gives 2nd and 3rd diagrams in 2nd factor of numerator. Conclusion: disconnected diagrams *cancel* in numerator & denominator. ("Linked cluster expansion": Brueckner 1955; Goldstone 1957).

- Green's function is sum of *connected* diagrams.

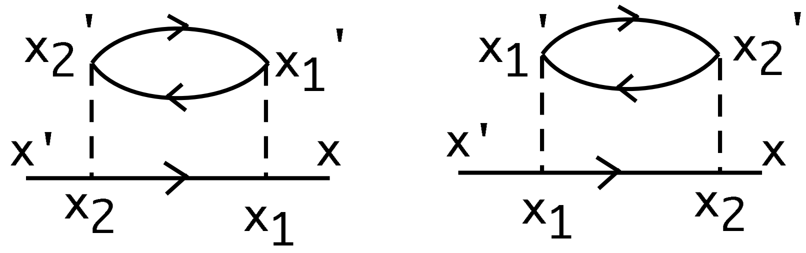
  Final result in diagrammatic form:



- Remarks on higher order diagrams:

  a) nth order term has n factors of v (dashed lines)

  b) $\star$ Counting: nth order term involves n dummy variables $\tau_1 \ldots \tau_n$. So we generate similar diagrams like



  which correspond to identical terms in the perturbation series

$$\int d^4x_1 d^4x_1' d^4x_2 d^4x_2' v(x_2 - x_2') v(x_1 - x_1') \times$$
$$\times G_0(x, x_1) G_0(x_1, x_2) G_0(x_2, x') G_0(x_1', x_2') G_0(x_2', x_1')$$

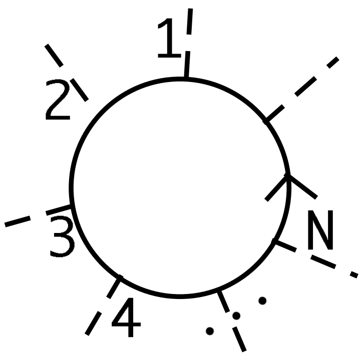
  and the identical term with $x_1, x_1' \leftrightarrow x_2, x_2'$.

  Exercise: convince yourself that the number of *topologically identical* diagrams of each type is $2^n n!$ (e.g., the ones above, where there are exactly 8 similar diagrams generated in the perturbation series!).[12] Convince yourself further that every diagram gives

[12]Hint: contract external index x with one of the internal indices, then ask how many remaining possibilities there are to contract x' with an internal index. Not all possibilities are allowed within a given class of diagram, since the $v(x_1 - x_2)$ factors restrict which remaining contractions give similar diagrams!

exactly the same contribution when evaluated. But $1/(2^n n!)$ is exactly the numerical prefactor in the pert. series, so we can *replace* the series (24) by one in which we count each *topologically distinct* picture only once, and forget prefactor $1/n!$ in Eq. (24) and $1/2^n$ from def. of V_I's.

c) How to account for - signs in evaluating diagrams? Note we pick up a minus sign in the diagrams we've looked at so far only when there is an odd number of *closed fermion loops*. This is because in general closed loop has form



$$\psi^\dagger(1)\ \psi(1)\ \psi^\dagger(2)\ \psi(2)\ \psi^\dagger(3)\ \psi(3)\ \cdots\ \psi^\dagger(N)\,\psi(N)$$

And there is always one minus sign from the necessity to commute the last Fermi operator with the first.

d) $\star$ When you see $G_0(x,x)$, it means $G_0(\mathbf{r},\tau,\mathbf{r},\tau^+)$, since fields at equal times always come from $\hat{V}_I(\tau)$, and therefore occur in order $\hat{\psi}^\dagger\hat{\psi}$.

- Momentum space perturbation theory:

For transl. invariant systems it's more convenient to look at the Green's function for a particle with momentum $\mathbf{p}$, $G(\mathbf{p})$.

Fourier transforms:

a) $G(\mathbf{r},\tau) = T\sum_n \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}-i\omega_n\tau} G(\mathbf{k},\omega_n)$

b) $v(\mathbf{r},\tau) = T \sum_{\text{n even}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}-i\omega_n\tau} v(\mathbf{k},\omega_n)$

(Only n even occurs, for fermions or bosons, since v is a bilinear operator. For instantaneous potentials, $v(\tau) \sim \delta(\tau)$, find $v(\mathbf{k},\omega_n) = v(\mathbf{k})$ only, using $\delta(\tau) = \sum_{\text{n even}} e^{-i\omega_n\tau}$)

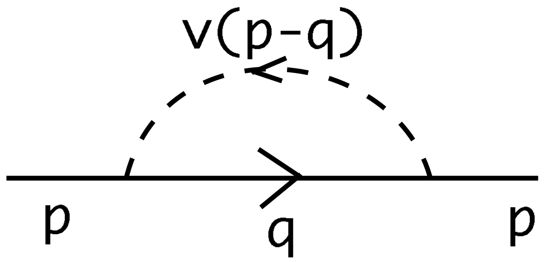
Now examine one of 1st-order terms in pert. series (diagram c)[13]

$$
\begin{aligned}
\overline{G}_1(x-x') &= \frac{Z_0}{2}\int d^4x_1 d^4x_2 v(x_1-x_2) G_0(x,x_1) G_0(x_2,x') G_0(x_1,x_2) \\
&= \frac{Z_0}{2}\sum_{\mathbf{k}\mathbf{k}'\mathbf{q}\mathbf{q}'} T^4 \sum_{nn'mm'} \int d^4x_1 d^4x_2 v(q') G_0(k) G_o(k') G_0(q) \times \\
&\quad \times e^{i[q'(x_1-x_2)+k(x-x_1)+k'(x_2-x')+q(x_1-x_2)]}
\end{aligned}
$$

so

$$
\begin{aligned}
\overline{G}(p) &= \int d^4(x-x') e^{-ip(x-x')} \overline{G}_1(x-x') \\
&= \frac{Z_0}{2}\sum_{\mathbf{k}\mathbf{k}'\mathbf{q}\mathbf{q}'} v(q') G_0(k) G_o(k') G_0(q) \times \\
&\quad \times \int d^4x_1 d^4x_2 d^4(x-x') e^{i(q'-k+q)x_1} e^{i(k'-q-q')x_2} e^{i(k-p)x} e^{i(p-k')x'} \\
&= \frac{Z_0}{2}\sum_{\mathbf{q}} v(p-q) G_0(p)^2 G_0(q)
\end{aligned}
$$

So this process looks like



and we see that one can think of the interaction line $v(p-q)$ as carrying momentum $p-q$, and momentum being conserved at each vertex.

[13] Recall since $k \equiv \mathbf{k},\omega_n$, $kx = \mathbf{k}\cdot\mathbf{r} - \omega_n\tau$.

3.2.5 Feynman rules

Feynman rules (in position space) for nth order contribution to G:

1. Draw all topologically distinct diagrams with n interaction lines and $2n+1$ directed particle lines.
2. Associate factor $G_0(1,2)$ to each line $2 \to 1$.
3. "" $V(1,2)$ with each interaction line $------$.
4. Integrate all internal variables $\int_0^\beta d\tau_a$.
5. Multiply each diagram by $(-1)^n(-1)^F$. (F is number of closed Fermi loops).
6. $G_0(x,x)$ interpreted as $G_0(\mathbf{r},\tau,\mathbf{r},\tau^+)$.
7. Spin: $G's$ are really matrices in spin space, so product is really matrix product in spin space,

$$G_0(1,2)G_0(2,3) \to \sum_{\sigma''} G_{0\sigma\sigma''}(1,2)G_{0\sigma''\sigma'}(2,3) \tag{37}$$

Feynman rules (in momentum space) for nth order contribution to G:

1. Draw all topologically distinct diagrams with n interaction lines and $2n+1$ directed particle lines.
2. Associate wave vector and matsubara frequency with each particle line and conserve at every vertex.
3. Associate factor $G_0(\mathbf{k},\omega_n) \equiv 1/(i\omega_n - \xi_\mathbf{k})$ to each line with "4-momentum" $\mathbf{k},\omega_n$
4. Each interaction line $-- > --$ should be directed and associated with $v(\mathbf{k})$
5. Integrate/sum over all internal momenta.
6. Multiply each diagram by $(-1)^n(-1)^F$.
7. Whenever a particle line closes on itself, insert convergence factor $e^{i\omega_n 0^+}$.[14]

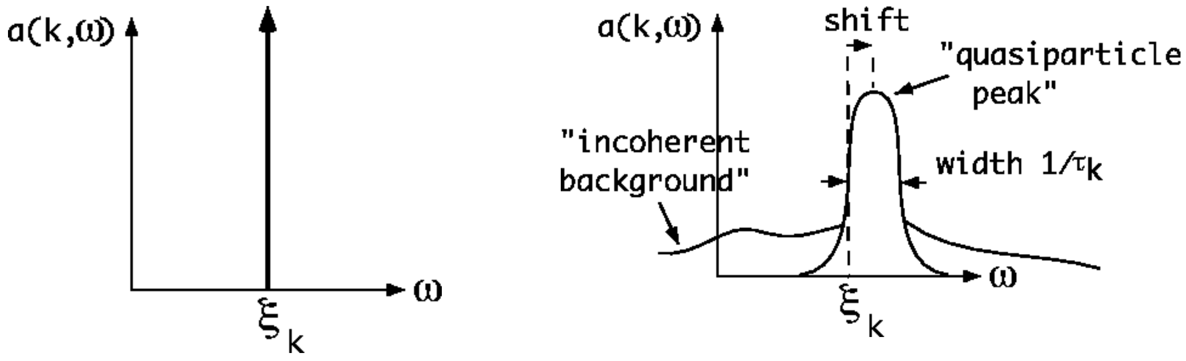
[14]forces completion of contours in uhp only, equivalent to 6) in real space rules.

8. Spin: evaluate matrix spin sums.

3.3 Dyson equation

3.3.1 Self-energy

Dyson reformulated the perturbation series for G basically by noting that one could consider all diagrams for G with external legs removed, and where you couldn't cut the diagram in the middle to produce two new valid diagrams, call it the *self-energy* Σ of the system, and express the exact G in terms of it in closed form. This approach is useful because σ has a more direct physical interpretation. In terms of our previous discussion in Sec. 2, for an interacting system we expect crudely that the pole at $\xi_{\mathbf{k}}$ in the noninteracting Green's function $G_0(\mathbf{k}, \omega_n) = (i\omega_n - \xi_{\mathbf{k}})^{-1}$ will be shifted and acquire an imaginary part:



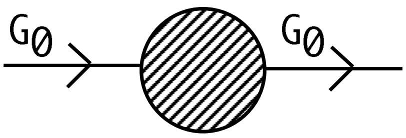
In fact in general Dyson shows us we can write

$$
\begin{aligned}
G^R(\mathbf{k}, \omega) &= \frac{1}{\omega + i0 - \xi_{\mathbf{k}} - \Sigma(\mathbf{k}, \omega)} && (38)\\
\mathrm{Re}\Sigma &\equiv \tilde{\xi}_{\mathbf{k}} - \xi_{\mathbf{k}} = \text{ shift of pole} && (39)\\
\mathrm{Im}\Sigma &\equiv \frac{1}{2\tau_{\mathbf{k}}} = \text{ relaxation rate} && (40)
\end{aligned}
$$

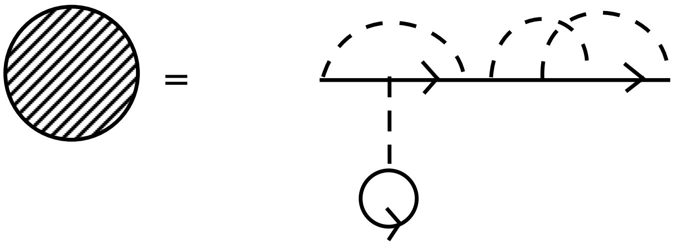
Note if (38) is true, the $Z_{\mathbf{k}}$ factor defined in the last section must emerge in some rather complicated way.

- General diagram for G:

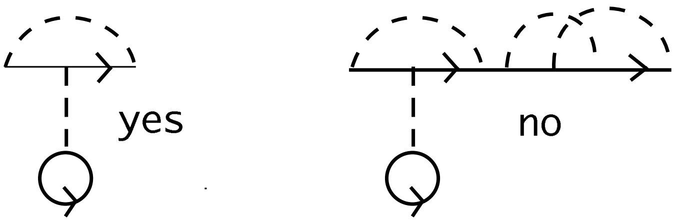
begins and ends with G_0:



where the blob in the middle represents some messy scattering process, e.g.



- Define *proper self-energy* Σ to be sum of all such diagrams which can't be cut into 2 valid pieces by cutting a G_0 line:



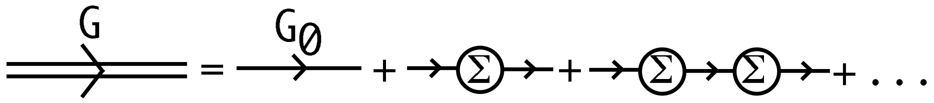
A diagram which can't be cut in this way is called *irreducible*, and sometimes the proper self-energy is referred to as the irreducible self-energy.

- Dyson point:

Any diagram for G is now to be found in the set

$$\left\{ \to\Sigma\to \,, \to\Sigma\to\Sigma\to \,, \to\Sigma\to\Sigma\to\Sigma\to\cdots \right\}$$

- But G is sum of all topologically distinct diagrams:

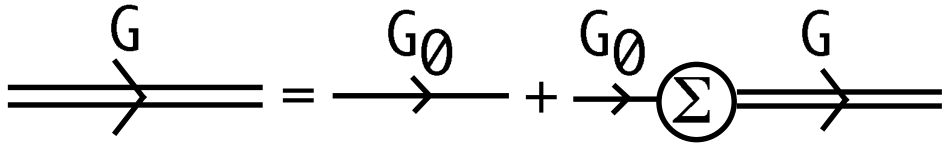


$$G(1;1') = G_0(1;1') + \int d2d2'\, G_0(1;2)\Sigma(2,2')G_0(2';1') + \ldots \tag{41}$$

Or, in F.T. rep. (transl. inv. systems!):

$$G(\mathbf{k},\omega_n) = G_0(\mathbf{k},\omega_n) + G_0(\mathbf{k},\omega_n)\Sigma(\mathbf{k},\omega_n)G_0(\mathbf{k},\omega_n) + \ldots \tag{42}$$

- Note products are simple products in Fourier transformed representation, all internal summations contained in Σ! Therefore can simply sum geometric series:



$$G(\mathbf{k},\omega_n) = \frac{G_0}{1 - G_0\Sigma} = \frac{1}{(G_0)^{-1} - \Sigma} = \frac{1}{i\omega_n - \xi_{\mathbf{k}} - \Sigma} \tag{43}$$

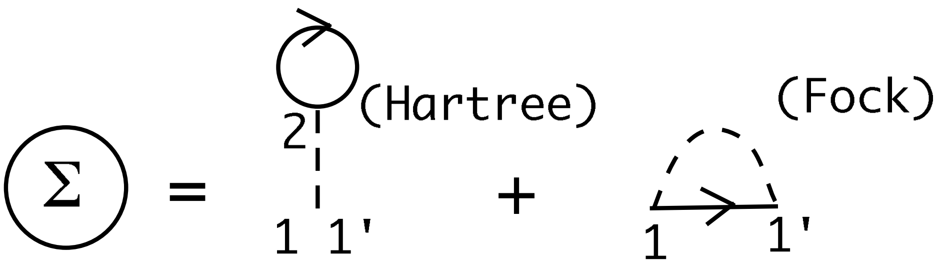
3.3.2 Approximations to self-energy:

In general interactions aren't weak, can't sum perturbation series for Σ exactly. But if we approximate Σ, Dyson expansion guarantees us an approximation which includes some diagrams to infinite order; frequently (but not always) a better approximation. Usually we need to justify a given approximation in any special case.[15]

[15]See Baym & Kadanoff (196?) for discussion of how to construct approximations for Σ which preserve physical conservation laws.

Examples:

- Hartree-Fock approximation: retain only 1st-order Feynman diagrams in self-energy:



so self-energy can be written (check!)

$$
\begin{aligned}
\Sigma(1';1) &= \mp\delta(1-1')\int_0^\beta d2\; v(1-2)G_0(2,2^+) - G_0(1',1)v(1-1') \\
&= \mp\delta(\tau_1-\tau_1')\delta(\mathbf{r}-\mathbf{r}')\int_0^\beta d\tau_2\int d^3r_2\delta(\tau_1-\tau_2)V(\mathbf{r}_1-\mathbf{r}_2)G_0(\mathbf{r}_2,\tau_2,\mathbf{r}_2,\tau_2^+) \\
&\quad -\delta(\tau_1-\tau_1')V(\mathbf{r}_1-\mathbf{r}_1')G_0(\mathbf{r}_1,\tau_1;\mathbf{r}_1',\tau_1') \\
&= \delta(\tau_1-\tau_1')\left(\delta(\mathbf{r}-\mathbf{r}')\int d^3r_2V(\mathbf{r}_1-\mathbf{r}_2)n(\mathbf{r}_2) - V(\mathbf{r}_1\mathbf{r}_1')G_0(\mathbf{r}_1,\tau_1;\mathbf{r}_1',\tau_1')\right)
\end{aligned}
$$

where I've used $G_0(\mathbf{r}_2,\tau_2,\mathbf{r}_2,\tau_2^+) = -\pm\langle\hat\psi^\dagger(\mathbf{r}_2)\hat\psi(\mathbf{r}_2)\rangle = \mp n(\mathbf{r}_2)$.

The Hartree (first) term can be seen to represent nothing but the average interaction energy, i.e. it's the interaction energy of the particle at 1 with a 2nd particle at 2, averaged over all space. Since $V(\mathbf{r}-\mathbf{r}')$ and $n(\mathbf{r})$ are real, this term in Σ is strictly real. The Fock, or exchange term looks more complicated since it involves the dynamics of the particle propagating from 1' to 1, but it is still instantaneous in time $\propto \delta(\tau-\tau')$. This means that the analytically continued (real time) self-energy will be frequency independent and real. For example, if we Fourier transform assuming translational invariance (check!), we find:

$$
\begin{aligned}
\Sigma(\mathbf{k},\omega_n) &= \int_0^\beta e^{-i(\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')-i\omega_n(\tau-\tau')}\Sigma(\mathbf{r}-\mathbf{r}';\tau-\tau') \\
&= V(\mathbf{q}=0)\sum_{\mathbf{k}} n(\mathbf{k}) \pm \sum_{\mathbf{k}'} n_{\mathbf{k}'}V(\mathbf{k}-\mathbf{k}')
\end{aligned}
$$

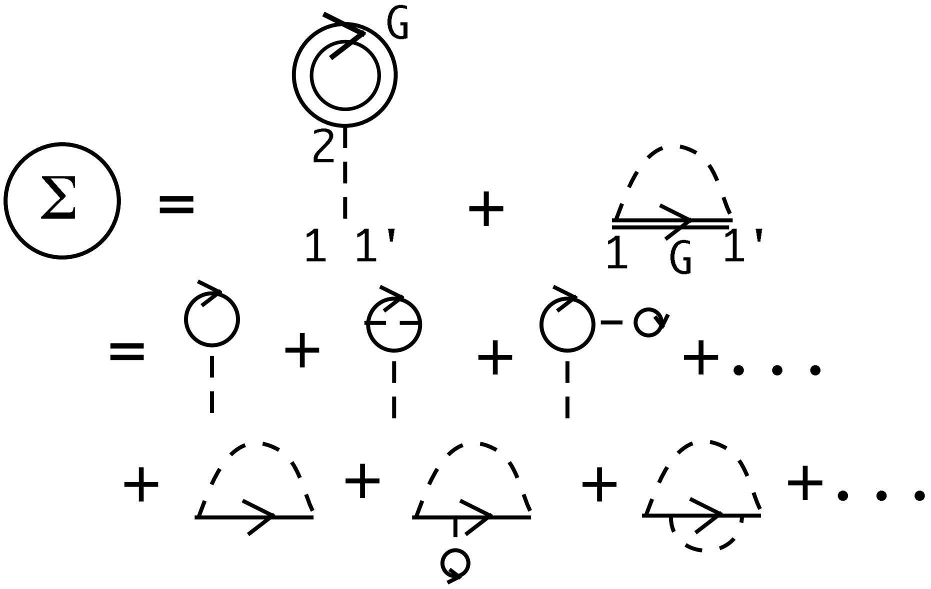
where $n_{\mathbf{k}} \equiv \langle a_{\mathbf{k}}^\dagger a_{\mathbf{k}}\rangle$ is the average number of particles with momentum $\mathbf{k}$.

Analytical continuation to the retarded self-energy, whose imaginary part gives the relaxation rate $\mathrm{Im}\Sigma^R(\mathbf{k},\omega) = -1/2\tau_k$, involves only replacing $i\omega_n \to \omega + i0^+$, according to the uniqueness theorem discussed at the end of Section 2. Since in the Hartree-Fock approximation $\Sigma(\mathbf{k},\omega_n)$ is ω_n independent, we have $\Sigma^R = \Sigma$. The Hartree (first) term in (44) is manifestly real and $\mathbf{k}-$ and $\omega-$ independent; therefore it will not contribute to the scattering rate $1/\tau_k$, and can in fact be ignored: aside from a shift of the chemical potential, it will have no physical consequences. The Fock (second) term involves the dynamics of a particle propagating in the intermediate state, but in fact is seen also to be real.[16] Thus Σ^R in this order simply involves a static, but **k**-dependent shift of the quasiparticle energies which may be thought of as the shift of their energies in the presence of the "molecular field" or "mean field" provided by the averaged interactions with the medium consisting of all the other particles.

- Self-consistent Hartree-Fock approximation

The approximation discussed above, while frequently employed and often very convenient for a quick estimate of the effect of interactions, may be shown to violate certain exact relations[17] between the one-particle Green's function which determine particle densities and the correlation functions which determine particle currents; in other words, conservation laws are violated. [18] A conserving approximation can be constructed with a similar philosophy by calculating the self-energy self consistently; i.e. Σ is taken to be a functional of G rather than G_0. Diagrammatically, this can be represented as:

[16]We assume $V(\mathbf{r}-\mathbf{r}') = V(|\mathbf{r}-\mathbf{r}'|)$, so that $V(\mathbf{q})$ is real.
[17]These relations are called Ward identities, which are beyond the scope of this course
[18]B&K, Phys. Rev. 124, (1961); K&B, *Quantum Statistical Mechanics, Benjamin Advanced Book Series.*



Let's return to the equation of motion for the Green's function in the presence of interactions, which looks like

$$\begin{aligned} &[\partial_{\tau_1} + h_0(\mathbf{r}_1)]G(1;2) \\ &\mp \int d1' v(1-1') G(1;\mathbf{r}_2,\tau_1;1';\mathbf{r}_2,\tau_1^+) \\ &\qquad = -\delta(1-2) \end{aligned} \tag{44}$$

with

$$G(1;2;3;4) \equiv \langle \mathcal{T}_\tau \left[\hat{\psi}(\mathbf{r}_1,\tau_1)\hat{\psi}(r_2,\tau_2)\hat{\psi}^\dagger(\mathbf{r}_3,\tau_3)\hat{\psi}^\dagger(\mathbf{r}_4,\tau_4) \right] \rangle \tag{45}$$

The two-particle Green's function in (44) would factorize if the $\hat{\psi}$'s were interaction picture operators (they're not!), or if $\hat{H} = \hat{H}_0$. We would then get

$$G_0(1;2;3;4) = G_0(1;4)G_0(2;3) \pm G_0(1;3)G_0(2;4) \tag{46}$$

This means the particles propagate independently without interactions (see Sec. 4). One might ask what the meaning of such a factorization would be if we used full G's:

$$\begin{aligned} G(1;2;3;4) &= G(1;4)G(2;3) \pm G(1;3)G(2;4) \oplus \text{ "correlations"} \\ &\simeq G(1;4)G(2;3) \pm G(1;3)G(2;4) \quad ? \end{aligned}$$

The word "correlations" then means any kind of effects of interactions between particles which are not subsumable in terms of an average molecular field which simply shifts the qp energies. If we neglect the correlations, as in the 2nd line of (47), the equation of motion reads

$$\begin{aligned}[\partial_{\tau_1} + h_0(\mathbf{r}_1)]G(1;2) &= -\delta(1-2) \\ &\pm \int_0^\beta d1' v(1-1')[G(1,1'_+)G(1',2) \pm G(1,2)G(1',1'_+)]_{\tau_1=\tau_1'}\end{aligned}$$

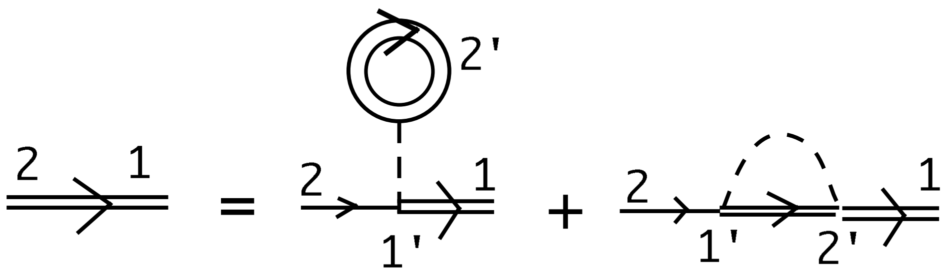
which can be integrated using the boundary condition corresponding to the noninteracting case

$$[\partial_{\tau_1} + h_0(\mathbf{r}_1)]G_0(1;2) = -\delta(1-2)$$

to find

$$G(1;2) = G_0(1-2) - \int_0^\beta d1'd2' G_0(1';2)v(1'-2')[G(1,1')G(2',2'_+) \pm G(2',1')G(1,2')]$$

which is just



So we can compare with the self-energy diagrams above and see that the factorization scheme above is consistent with a choice of self-energy equivalent to the self-consistent Hartree-Fock diagrammatic approximation above Eq. (44). Note it contains an infinite number of Feynman diagrams (where G_0 is the building block), making it a *partial resummation* of perturbation theory (partial because diagrams not of the Hartree or Fock type are not included). It may also be thought of as an approximation of two *skeleton* diagrams (based on the building block G). The problem of finding G is not solved by (47), of course, since the equation involves G on both the left and right-hand sides. Typically numerical methods are employed to solve (47), yielding for example energy bands in solids in which Coulomb interactions among electrons have been included in the simplest possible average way. Such methods break down for condensed matter systems where interactions (more properly, correlations) are strong.

3.3.3 Validity of Hartree-Fock theory

Crucial question: when is such an approximation—taking only the 1st order term in the self-energy—a good one for an interacting system? The answer, curiously, turns out to be different for bosons and fermions. The HF approximation is a good one for interacting *low density Bose systems* or *high density Fermi systems*!

Intuitively it seems obvious that if the particles are further apart on the average, they will interact less strongly and less often, so a mean field theory like Hartree-Fock theory should work well. This is true in the Bose case: the only characteristic energies are the temperature T and the zero-point energy. The latter is just the energy scale obtained by confining the particle to a cage of size the interparticle spacing r_s, i.e. $\hbar^2/(2mr_s^2)$. The interaction is typically characterized by a *strength* V and a *range* a, and if $r_s \gg a$, the particles don't feel the potential much and the ground state energy, for example, of such a gas can be expanded at $T = 0$ in powers of a/r_s. The result is

$$E_0 = E_0^{HF} + E_{corr} \tag{47}$$

with E_0^{HF} the ground state energy calculated in the independent particle approximation with the Hartree-Fock energy shifts, and E_{corr} the *correlation energy*, which is found to vary as

$$\frac{E_{corr}}{E_0^{HF}}(a/r_s)^{\alpha}, \text{ (bosons)} \tag{48}$$

with $\alpha = xxx$, and therefore $\to 0$ in the low density limit. In the case of long-range interactions, can this argument be made???

In the case of Fermions, a new energy scale arises due to the Pauli principle, namely ε_F. As the density increases, so does ε_F, which represents the average kinetic energy of electrons; this increase is faster than the increase of the correlation energy. For the electron gas with Coulomb interactions, for example, we have, in terms of the Bohr radius a_0 we have (per particle)

$$K.E. = \tfrac{3}{5}\varepsilon_F = \frac{2.21}{(r_s/a_0)^2}\ \mathrm{Ryd} \tag{49}$$

$$P.E.|_{HF} = \frac{-0.916}{(r_s/a_0)}\ \mathrm{Ryd} \tag{50}$$

and the correlation energy is given by

$$\frac{E_{corr}}{\varepsilon_F} = 0.0622 \log \frac{r_s}{a_0} - 0.096 + \ldots \tag{51}$$

so it is clear the correlation term is less singular than the HF term in the limit $r_s \to 0$. At higher densities, particles are effectively independent.