Diagrams....

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I. FEYNMAN RULES IN MOMENTUM-FREQUENCY SPACE

For a homogeneous system, the one-particle Green's function

$$\mathcal{G}(\mathbf{r},\tau) \equiv \mathcal{G}(\mathbf{r}_1,\tau_1;\mathbf{r}_1+\mathbf{r}\tau_1+\tau) = \begin{cases} -\left\langle e^{\tau(H-\mu N)}\Psi(\mathbf{r}_1+\mathbf{r},0)e^{-\tau(H-\mu N)}\Psi^\dagger(\mathbf{r}_1,0)\right\rangle, & \text{for } \tau>0 \\ \mp\left\langle e^{-\tau(H-\mu N)}\Psi^\dagger(\mathbf{r}_1,0)e^{\tau(H-\mu N)}\Psi(\mathbf{r}_1+\mathbf{r},0)\right\rangle, & \text{for } \tau<0 \end{cases} \tag{1}$$

can be diagonalized in Fourier space

$$\mathcal{G}(\mathbf{k},i\omega_n) = \int_0^\beta d\tau \int d\mathbf{r}\, e^{i(\omega_n\tau-\mathbf{k}\cdot\mathbf{r})}\,\mathcal{G}(\mathbf{r},\tau) \tag{2}$$

$$\mathcal{G}(\mathbf{r},\tau) = \frac{1}{\beta}\sum_n \frac{1}{V}\sum_{\mathbf{k}} e^{-i(\omega_n\tau-\mathbf{k}\cdot\mathbf{r})}\,\mathcal{G}(\mathbf{k},i\omega_n) \tag{3}$$

$$= T\sum_n \int \frac{d\mathbf{k}}{(2\pi)^D}\, e^{-i(\omega_n\tau-\mathbf{k}\cdot\mathbf{r})}\,\mathcal{G}(\mathbf{k},i\omega_n) \tag{4}$$

where we have taken the thermodynamic limit replacement $V^{-1}\sum_{\mathbf{k}} \to \int d\mathbf{k}/(2\pi)^D$ the limit of large volume V in D dimensions. The summation over Matsubara frequencies, ω_n, goes over all integers with

$$\omega_n = \begin{cases} 2n\pi T, & \text{Bosons} \\ (2n+1)\pi T, & \text{Fermions} \end{cases} \tag{5}$$

Notice that the summation over frequencies for finite temperature $T = 1/\beta > 0$ is similar to the summation over k-space in a calculation of finite volume V. In the limit of zero temperature, $T \to 0$, the summation over discrete frequency will go over to an integral, similar to the thermodynamic limit expressions in k-space.

In Fourier space, the inverse of the non-interacting Greens function has the same, simple form for Bosons as for Fermions

$$\mathcal{G}_0^{-1}(\mathbf{k},i\omega_n) = i\omega_n + \mu - \varepsilon_k \tag{6}$$

where $\varepsilon_k = \hbar^2k^2/2m$ are the free particle energies.

We now want to write down the expressions of any Feynman diagrams, whose rules have been given in real space - imaginary time before, in Fourier space. For this, we need the Fourier expression of the interaction potential

$$v(\mathbf{k}) = \int d\mathbf{r} e^{-i\mathbf{k}\cdot\mathbf{r}} v(r) \tag{7}$$

$$v(\mathbf{r}) = \int \frac{d\mathbf{k}}{(2\pi)^D}\, e^{i\mathbf{k}\cdot\mathbf{r}} v(k) \tag{8}$$

instantaneous in imaginary time, e.g.

$$\int d\tau \int d\mathbf{r}\, e^{i(\omega_n\tau-\mathbf{k}\cdot\mathbf{r})} v(\mathbf{r})\delta(\tau) = v(k) \tag{9}$$

A general interaction vertex involves the expressions

$$\int_0^\beta d\tau \int d\mathbf{x}_1 \int d\mathbf{x}_2 \, \mathcal{G}_0(\mathbf{r}_1,\tau_1;\mathbf{x}_1,\tau)\mathcal{G}_0(\mathbf{r}_2,\tau_2;\mathbf{x}_2,\tau)v(|\mathbf{r}_1-\mathbf{r}_2|)\mathcal{G}_0(\mathbf{x}_1',\tau;\mathbf{r}_1',\tau_1')\mathcal{G}_0(\mathbf{x}_2,\tau;\mathbf{r}_2',\tau_2') \tag{10}$$

$$= \int_0^\beta d\tau \int d\mathbf{x}_1 \int d\mathbf{x}_2 \int \frac{d\mathbf{k}}{(2\pi)^D} e^{i\mathbf{k}\cdot(\mathbf{x}_2-\mathbf{x}_1)}$$

$$\times T\sum_{n_1}\int \frac{d\mathbf{k}_1}{(2\pi)^D} e^{-i(\omega_{n_1}(\tau-\tau_1)-\mathbf{k}_1(\mathbf{x}_1-\mathbf{r}_1))}\mathcal{G}_0(\mathbf{k}_1,n_1) \quad T\sum_{n_2}\int \frac{d\mathbf{k}_2}{(2\pi)^D} e^{-i(\omega_{n_2}(\tau-\tau_2)-\mathbf{k}_2(\mathbf{x}_2-\mathbf{r}_2))}\mathcal{G}_0(\mathbf{k}_2,n_2)$$

$$\times T\sum_{n_1'}\int \frac{d\mathbf{k}_1'}{(2\pi)^D} e^{i(\omega_{n_1'}(\tau-\tau_1')-\mathbf{k}_1'(\mathbf{x}_1-\mathbf{r}_1'))}\mathcal{G}_0(\mathbf{k}_1',n_1')T\sum_{n_2'}\int \frac{d\mathbf{k}_2'}{(2\pi)^D} e^{i(\omega_{n_2'}(\tau-\tau_2')-\mathbf{k}_2'(\mathbf{x}_2-\mathbf{r}_2'))}\mathcal{G}_0(\mathbf{k}_2',n_2') \tag{11}$$

We can see that the imaginart time integration over τ only contributes if $n_1+n_2=n_1'+n_2'$ with a factor β as well as the $\mathbf{x}_1$ integration leads to $\mathbf{k}_1'=\mathbf{k}+\mathbf{k}$ as well as $\mathbf{k}_2'=\mathbf{k}_2-\mathbf{k}$ from the $\mathbf{x}_2$ integration.

Therefore, total momenta as well as total Matsubara frequencies of incoming lines have to be conerved at an interaction vertex and equal the outgoing ones.

We then get the general rules of Feynman diagrams in frequency space of order n

- draw all connected, topologically disting diagrams involving n interaction vertices as before in real space
- instead of associating space and imaginary time, associate momenta and frequencies to each line. External lines have the same external momenta and frequency, whereas for internal lines they have to satisfy conservation of momenta and frequency at each interaction vertex (sum of incoming momenta/frequancy must equal sum of outcoming momenta/frequency).
- With each solid (propagator) line of momentum $\mathbf{k}$ and frequency ω_n associate the non-interacting Green's function $\mathcal{G}_0(\mathbf{k},i\omega_n)=[i\omega_n+\mu-\varepsilon_{\mathbf{k}}]^{-1}$.
- with each wavy (interation) line associate $-Tv(\mathbf{q})/(2\pi)^D$ where $\mathbf{q}=\mathbf{k}_2-\mathbf{k}_1$ is the difference of the two incoming momenta.
- Integrate over all internal (independent) momenta and sum over all frequencies ($\omega_n=2\pi nT$ for bosons and $\omega_n=(2n+1)\pi T$ for fermions, $n=0,\pm1,\pm2,\dots$).
- multiply the expression by $(\mp1)^F$ where F is the number of Fermion loops.
- In case of non zero spin, s, for a spin-independent Hamiltonian, the summation over internal spin states gives an additional factor $of(2s+1)^F$.
- Insert $e^{i\omega_n\epsilon}$ with $\epsilon\to+0$ in cases the frequency summation is not absolutely convergent (only needed in particular subgraphs, enforces original operator ordering in the interaction).

A. Summing Matsubara frequencies

We need a basic method to evaluate summation over Matsubara-frequencies $\omega_n=\pi(2n+1)T$ for $n=0,\pm1,\dots$

$$\sum_n g(\omega_n) = -\frac{\beta}{2\pi i}\lim_{\tau\to0}\int_C e^{\omega\tau}f_F(\omega)g(\omega)d\omega \tag{12}$$

$$f_F(\omega) = \frac{1}{e^{\beta\omega}+1} \tag{13}$$

where the integral is in the complex planes with a contour C going around each pole of the Fermi-function $f_F(\omega)$ at $\omega=\omega_n$ in the positive sense. If we know the analytic properties, we can deform the contour to evaluate the Matsubara summation. (The $e^{i\omega0+}$-factor is often there, but not explicitly written down.)

Simple branch cut on the real axis. Suppose that $g(\omega)$ is analytic in the upper/ lower complex plane, but with simple poles on the real axis. Further, $g(\omega)$ vanishes for $|\omega|\to\infty$. We can deform now the integration contour into two half-circles, one in the upper complex plane, one in the lower complex plane. The Fermi function assures

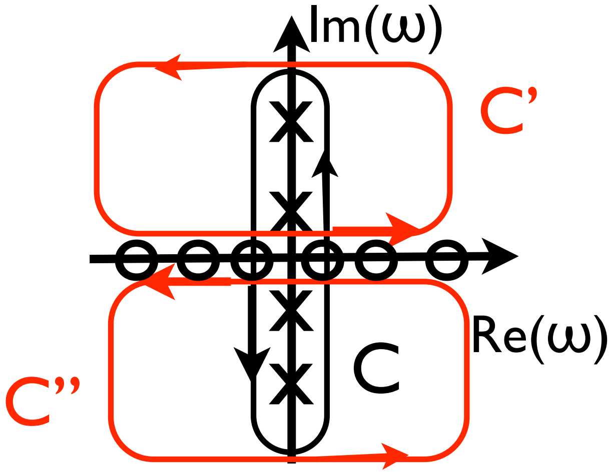


FIG. 1: A deformation of the contour integration C to C' and C''. Crosses are the Matsubara frequencies, the poles of the Fermi-function, whereas circles indicate possible poles (or a branch cut) of the original function. Note that C' is just above and C'' just below the real axis.

that the integration at infinity with positive real part of ω is neglegible, whereas the $e^{\omega 0^+}$ is needed to neglect the contributions at infinity for negative real part of ω. Only both integral close to the real axis contribute

$$T\sum_n g(i\omega_n) \;=\; -\frac{1}{2\pi i}\int_{-\infty}^{\infty} d\omega d\omega e^{\omega 0^+} f_F(\omega)\left[g(\omega+i\eta)-g(\omega-i\eta)\right] = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi} d\omega e^{\omega 0^+} f_F(\omega)A(\omega) \tag{14}$$

where we introduced the spectral function

$$A(\omega) = -\mathrm{Im}\, g(\omega+i\eta) \tag{15}$$

The spectral function is a fundamental quantity, since it occurs in many expressions. In the case of free fermions, we have $G_0(k,\omega_n)^{-1} = i\omega_n + \mu - k^2/2m$. The analytic continuation for ω away from the real axis is simple given by replacing $i\omega_n$ by ω. The spectral function is then

$$A_0(k,\omega) = 2\pi\delta(\omega - k^2/2m + \mu) \tag{16}$$

using the formal identity $1/(x+i\eta) = P/x - i\pi\delta(x)$. Putting the spectral function of the ideal Fermi gas bacl into the expression (14), we recover the density of the ideal Fermi gas. Note, that we could have also used different contours to evaluate the Matsubara summation leading to the same final result.

B. RPA-approximation

For Coulomb interacting particles, $v(r) = 1/r$ or $v(q) = 4\pi/q^2$ $(D=3)$, the divergence of the Coulomb potential $r \to 0$ or $q \to 0$ in general leads to divergent expressions in the perturbation series (look at Hartree-Fock and ladder diagrams in the figures below and identify potential divergencies!). Within the Green's function approach, we can analyse the potentially diverging diagrams. We can see that the bubble-diagrams, $B(q)$, can be dangereous, as thay occur in the form $[-v_q B_0(q)]^n$, with an arbitrary high power n. In the case, where the simple bubble $B_0(q)$ is finite at $q \to 0$, we are forced to include a whole series in order to avoid divergence. The resummation of this series is the RPA approximation in the diagrammatic approach.

Bubble diagram. Let us calculate the basic bubble diagram

$$B_0(\mathbf{k}, i\omega_n) \;=\; T\int\frac{d\mathbf{p}}{(2\pi)^3}\sum_m G_0(\mathbf{p}+\mathbf{k}, i\omega_{m+n})G_0(\mathbf{p}, i\omega_m) \tag{17}$$

$$= \int\frac{d\mathbf{p}}{(2\pi)^3}\int_C\frac{d\omega}{2\pi i} f_F(\omega)\frac{1}{\omega+2\pi i n T+\mu-\varepsilon_{\mathbf{k}+\mathbf{p}}}\frac{1}{\omega+\mu-\varepsilon_p} \tag{18}$$

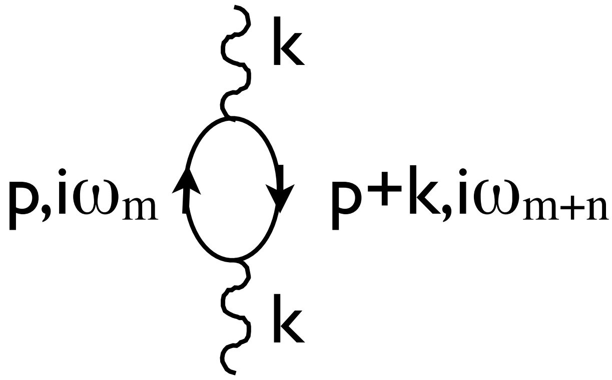


FIG. 2: The basic bubble diagram.

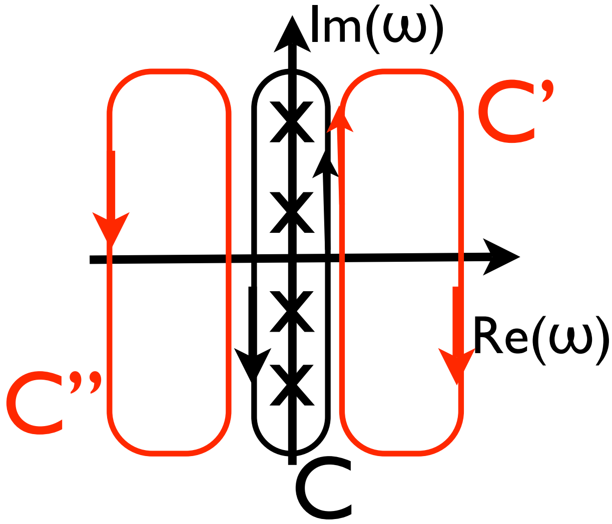


FIG. 3: A different deformation of the contour integration which we use to calculate the bubble diagram.

We can deform the contour and close it to the right and to the left, separately. The contributions from the half-circles with $|\omega| \to \infty$ vanishes, and we have only to take into account the two poles at $\omega = \varepsilon_{\mathbf{k}+\mathbf{q}} - \mu - 2\pi nT$ and at $\omega = \varepsilon_p - \mu$. We get

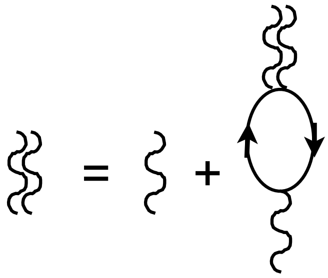
$$B_0(\mathbf{k}, i\omega_n = 2\pi i n T) \;=\; \int \frac{d\mathbf{p}}{(2\pi)^3} \frac{f_F(\varepsilon_p - \mu) - f_F(\varepsilon_{\mathbf{k}+\mathbf{p}} - \mu)}{i\omega_n + \varepsilon_p - \varepsilon_{\mathbf{p}+\mathbf{k}}} \tag{19}$$

where we have used that $f(\omega + 2\pi nT) = f(\omega)$. Note that the bubbles is now bosonic, concerning at least the Matsubara-index! Just note that we have treated the spin-polarized case, for unpolarized electrons the bubble result has to be multiplied by a factor of 2.

Screened Coulomb interaction - RPA summation. We can now analyse the bubble diagram in the limit $k \to 0$ in order to estimate the order of the divergence higher order perturbation terms invoving the structure $[-v_q B_0(q)]^n$. For zero Matsubara frequency,

$$B_0(k \to 0, 0) = \lim_{k \to 0} \int \frac{d\mathbf{p}}{(2\pi)^3} \frac{f_F(\varepsilon_p - \mu) - f_F(\varepsilon_{\mathbf{k}+\mathbf{p}} - \mu)}{\varepsilon_p - \varepsilon_{\mathbf{p}+\mathbf{k}}} = -\beta \int \frac{d\mathbf{p}}{(2\pi)^3} \frac{df_F(\varepsilon_{\mathbf{k}} - \mu)}{d(\beta\mu)} = -\frac{dn}{d\mu} \tag{20}$$

and we get a finite negative number, proportional to the compressibility of the free Fermi gas. At zero temperature



$$v_{eff}(q)=v(q)+v(q)B_0(q)\ v_{eff}(q)$$

FIG. 4: The RPA approximation for the effective interaction.

it reduces to the density of states at the Fermi level, k_F. For any finite Mastubara frequency, $B_0(k, i\omega_n \neq 0) \sim k^2$. Therefore we get singularities of order $[-v(q)B_0(q)]^n \sim 1/q^{2n}$ from a chain of n bubbles. However, it is bossible to include the bubbles sum up to all order, introducing the effective potential

$$v_{eff}(q) = v_q - v_q B_0(q,0) + [v_q B_0(q,0)]^2 - \cdots = \frac{v_q}{1 - v_q B_0(q,0)} \tag{21}$$

For $q \to 0$, we obtain a screened Coulomb potential in three dimensions,

$$v_{eff}(q) \to \frac{4\pi e^2}{q^2 + k_s^2}, \quad k_s^2 = 4\pi e^2 (dn/d\mu) \tag{22}$$

Two-Particle Green's function, Dielectric function. The bubble-diagram contains a particle-hole propagator which represents a vertex contribution to the two-particle Green's function. Schematically we have

$$G^{(2)}(1,2;1',2') = G(1,1')G(2,2') - G(1,2')G(2,1') + G(1,A)G(2,B)\Gamma(A,B;A',B')G(A',1')G(B',2') \tag{23}$$

The RPA summation can be seen as the following approximation for the vertex Γ,

$$\Gamma = v + vB_0\Gamma \tag{24}$$

which leads to the screened interaction $\Gamma = v/(1 - vB_0) = 1/(v^{-1} - B_0)$. It is straightforward to see, that an external potential will be also screened. A particular form of the two-particle Green's function is the density-density correlation function, from which the dielectric function can be determined.

The so-called RPA-approximation introduces another class of diagrams which are conviniently expressed by an effective interaction V_{eff} which includes the effect of repeated density-fluctuations

$$V_{eff}(1,2;1',2') = v(1-2) + v(1-2)\mathcal{G}(1,\bar{1})\mathcal{G}(2,\bar{2})v_{eff}(\bar{1},\bar{2};1',2') \tag{25}$$

The corresponding diagrams are particularily important for long-range (Coulomb) interactions where they lead to an effective screened potential. A rearrangement of the perturbation theory in terms of the effective screened potential is possible and gives finite results in the dilute limit, for example in the electron-gas.

C. Hartree-Fock

There are certain classes of diagrams which can be summed up easily. We will see that it is quite often neccessary to treat the diagrams inside these classes consistently in order to obtain a better behaved perturbation expansion in renormalized parameter space. In the folllowing we will consider Bose systems, however, most of the analysis can be extended to Fermions.

Hartree-Fock. The mean-field Hartree-Fock equations are obtained by the following approximation for the self-energy

$$\Sigma_{HF}(\mathbf{k}) = -T\sum_{n'}\int \frac{d\mathbf{p}}{(2\pi)^3}\left[v(0)\mathcal{G}_{HF}(p,\omega'_n) \pm v(|\mathbf{p}-\mathbf{k}|)\mathcal{G}_{HF}(p,\omega'_n)\right] \tag{26}$$

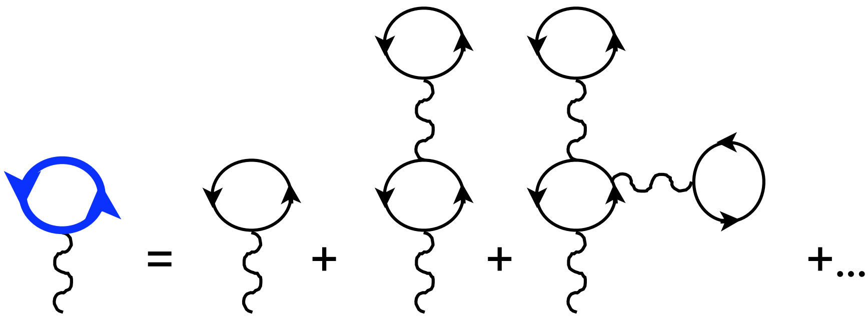


FIG. 5: The direct term of the self-energy in the Hartree-Fock approximation and its expansion in bare propagators.

where the minus sign accounts for fermions (1 momentum loop for the exchange part) and $\mathcal{G}_{HF}$ is the full propagator within this approximation

$$\mathcal{G}_{HF}^{-1} = G_0^{-1} - \Sigma_{HF} \tag{27}$$

Note that the self-energy is independant of ω_n in this approximation. Let us for the moment consider a bosonic system where the interaction potential is sufficiently weak, and does not depend on momentum (at least in the energy-region considered), $v(p) \simeq v(0) \equiv g$. In that case the self-energy is also momentum independant and is proportional to the density

$$\Sigma_{HF} = 2gn_{HF} \tag{28}$$

$$n_{HF} = -T\sum_n \int \frac{d\mathbf{p}}{(2\pi)^3}\mathcal{G}_{HF}(p,\omega_n) \tag{29}$$

$$= \int \frac{d\mathbf{p}}{(2\pi)^3}\frac{1}{e^{\beta(\varepsilon_p+\Sigma_{HF}-\mu)}-1} \tag{30}$$

$$= \lambda^{-3} g_{3/2}\left(e^{\beta(\mu-\Sigma_{HF})}\right) \tag{31}$$

Notice that the summation over Matsubara frequencies does not converge, as it is written. Since the field operator in the interaction operator are normal ordered, we have to insert a convergence factor which enforces normal ordering in the perturbation expansion, whenever the imaginary time difference between two operators is zero. Zero imaginary time difference is identical to a summation over Matsubara frequencies as encountered in the Hartree-Fock diagrams. The convergence factor must ensure normal ordering in the propagator, so that the summation over Matsubara frequencies just leads to the usual Bose/Fermi occupation number.

Bose-Einstein condensation is reached in this approximation when $\mu = \Sigma_{HF}$, which is a selfconsistent equation for μ. Let us approach the phase transition, setting $\Sigma_{HF} - \mu \to 0^+$. We have $g_{3/2}(e^x) \simeq 2.61 - 3.54\sqrt{-x}$, $n_{HF} \sim \mathcal{O}(1)$, and therefore $\Sigma_{HF} \sim \mathcal{O}(g)$ is linear in the coupling constant of the interaction. However, due to the non-analytic behavior of the $g_{3/2}$, the region of validity of any Taylor expansion around $\Sigma_{HF} - \mu = 0$ is zero.

What do we get if we would have started with the strict (not self-consistent) perturbation expansion? The first and second order terms included by the Hartree-Fock analyis are

$$\Sigma_{HF}^{(2)} = -2g\sum_n \int \frac{d\mathbf{p}}{(2\pi)^3}\mathcal{G}_0(\mathbf{p},n)\left\{1 - gT\sum_{n'}\int \frac{d\mathbf{p}'}{(2\pi)^3}[\mathcal{G}_0(\mathbf{p}',n')]^2\right\} \tag{32}$$

Now the second term inside the bracket on the rhs behaves roughly like the derivative of the bare density with respect to μ, and we see that the mean-field actually contains a summation of a series in $g/|\beta\mu|^{1/2}$. If we want to approach the point of $|\mu| \to 0$ higher orders in the perturbation theory diverge even more strongly. In our case, these problems occur do to so-called "infrared divergencies": in the limit of $\mu \to 0$, $\mathcal{G}(k,0) \sim \mu - k^{-2}/2m$ The Green's function approach allows us to estimate by simple dimensional analysis the effect of these infrared divergencies looking at the stricture of the integrals. We can see that the simple Hartree-Fock resummation cures the most diverging part, however, as soon as $\beta(\mu - \Sigma) \sim g^2$ additional diagrams have to be considered. Therefore, mean-field can be trusted outside this "critical region".

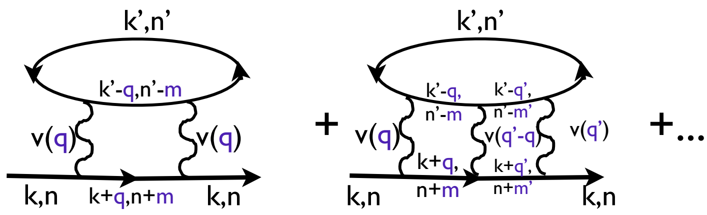


FIG. 6: Ladder diagrams.

Infrared problems are typical for phase-transitions, the renormalization group methods have developped powerful tools to "control" these problems. However, they all rely on basic assumptions on the (perturbative) analytic structure of the propagators.

D. T-matrix

We have seen that diagrams can help out to figure out potentially divergent subseries in the perturbation expansion. When treating hard-core-like potentials, we are expecting $v(q) \approx v(0)$ for $q \lesssim k_c$ with k_c large compared to typical momenta of the problems. Let us consider the so-called ladder diagrams shown in Fig. 6. The basic structure involved in the second order diagram contains

$$-T\sum_m \int \frac{d^3q}{(2\pi)^3} v(q)\mathcal{G}_0(k+q, i\omega_{n+m})\mathcal{G}_0(k'-q, i\omega_{n'-m}) \tag{33}$$

Since $\mathcal{G}_{,}^{-1}(q, i\omega_m) = \mu + i\omega_m - q^2/2m$, the integrand decays only as $1/q^4$ for large q, the momentum integral in 3d together with the frequency summation might not converge at large values for constant $v(q) \approx v(0)$. Indeed for large momenta and frequencies transfer $(q, m \to \infty)$, we have

$$\begin{aligned} -T\sum_m \int \frac{d^3q}{(2\pi)^3} v(q) \frac{1}{i\omega_m - q^2/2m}\frac{1}{-i\omega_m - q^2/2m} &= -T\sum_m \int \frac{d^3q}{(2\pi)^3} v(q)\frac{1}{\omega_m^2 + q^4/4m^2} \\ \approx -\int \frac{d^3q}{(2\pi)^3} v(q)\int d\omega \frac{1}{\omega^2 + q^4/4m^2} &= -\int \frac{d^3q}{(2\pi)^3}\frac{2mv(q)}{q^2}\int dy \frac{1}{y^2+1} \sim 2mv(0)k_c \end{aligned} \tag{34}$$

where k_c is the cut-off in momentum space, $v(q \gtrsim k_c) = 0$. We encouter the same problems as in two-body scattering theory! The divergent diagrams for $k_c \to \infty$ all have the structure of our basic diagram, those contained in the ladder diagrams correspond to the passage from the bare potential to the scattering length.

A different series which can be treated and which is potentially divergent for short range potentials (particularly hard-core), is related to the two-particle scattering problem. Let us consider particle-particle scattering. In terms of Green's function this is most easily done in terms of the two-particle Green's function $\mathcal{G}_2(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}'_1, \mathbf{r}'_2; \tau)$, defined as the average over two annihilation and two creation operators. Repeated particle-particle scattering can be written as a self-consistent equation for $\mathcal{G}_2$ in a matrix notation (numbers occuring twice are integrated over)

$$\mathcal{G}_2(1,2;1',2') \;=\; \mathcal{G}(1,1')\mathcal{G}(2,2') + \mathcal{G}(1,2';\tau)\mathcal{G}(2,1') + \mathcal{G}(1,\bar{1})\mathcal{G}(2,\bar{2},4)V(\bar{1},\bar{2})\mathcal{G}_2(\bar{1},\bar{2};1',2') \tag{35}$$

In the limit of $\beta\mu \to -\infty$ the system is dilute and the equation will include only two-particles scattering which each other. The two-body problem is solved by the complex T-matrix. For a dilute system G_2 can be replaced by the twi-body T-matrix which includes already repeated particle-particle scattering events. The on-shell T-matrix can be expressed in terms of the phase shifts, and in particular at low energies it reduces to a constant $4\pi\hbar^2 a/m$ where a is the scattering length.

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