Advanced Quantum Mechanics

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Lecture #23

Path Integrals and QM

Recap of Last Class

- Wick's Theorem and n-point correlators in imaginary time

- Perturbation theory for Z with x^4 potential.

- Feynman diagrams and Feynman rules

- Z upto 3rd order in pert. theory

- Connected and Disconnected Diagrams: Expansion for Free Energy

Linked Cluster Theorem and Replica Trick

We want to show that if we work out a perturbation series for F rather than Z, the contribution of disconnected diagrams drop out at each order.

$$Z^n = e^{n \ln Z} = 1 + n \ln Z + \sum_{m=2}^{\infty} \frac{(n \ln Z)^m}{m!} \qquad \ln Z = Lim_{n \to 0} \frac{d}{dn} Z^n$$

Now consider the following way of calculating Z^n :

Consider the partition function for n identical copies of the system. The copies do not talk to each other.

$$(Z)^n = \prod_\sigma \int \mathcal{D}[x^\sigma(\tau)] e^{-S_E[x^\sigma(\tau)]}$$

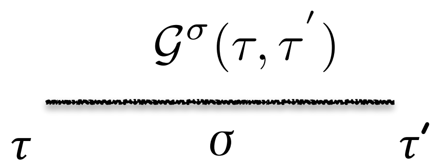
index σ denotes the copy and runs from 1 – n

Now, one can write down the perturbation expansion for $(Z/Z_0)^n$ in terms of Feynman diagrams including all the n x_σ variables.

It is clear that the diagrams whose contribution is linear in n would finally contribute to the perturbation expansion for F= $(1/\beta)$ ln Z.

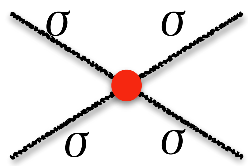
Linked Cluster Theorem and Replica Trick

Constructing Feynman Diagrams for $(Z/Z_0)^n$



Each line (2-pt fn) carries a σ index

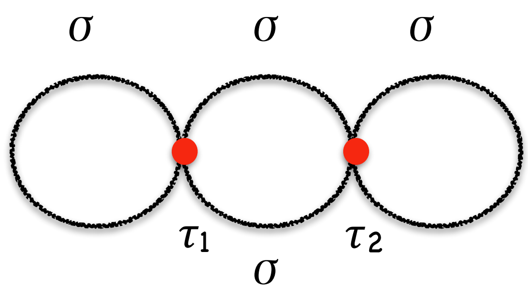
-g/4



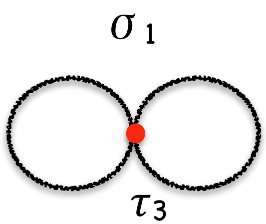
The 4 lines coming out of a vertex must carry the same σ index

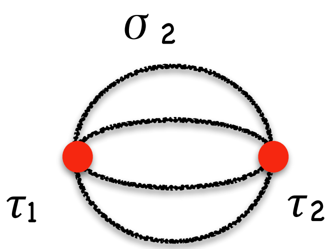
Remaining rules are same as for (Z/Z_0)

#1) A connected diagram has all lines with same σ index



#2) Consider a diagram with n_c disconnected clusters





#3) On top of the usual "multiplicities" or "Symmetry factors" of these diagrams for (Z/Z_0), each cluster has a σ index, which gives a factor of n.

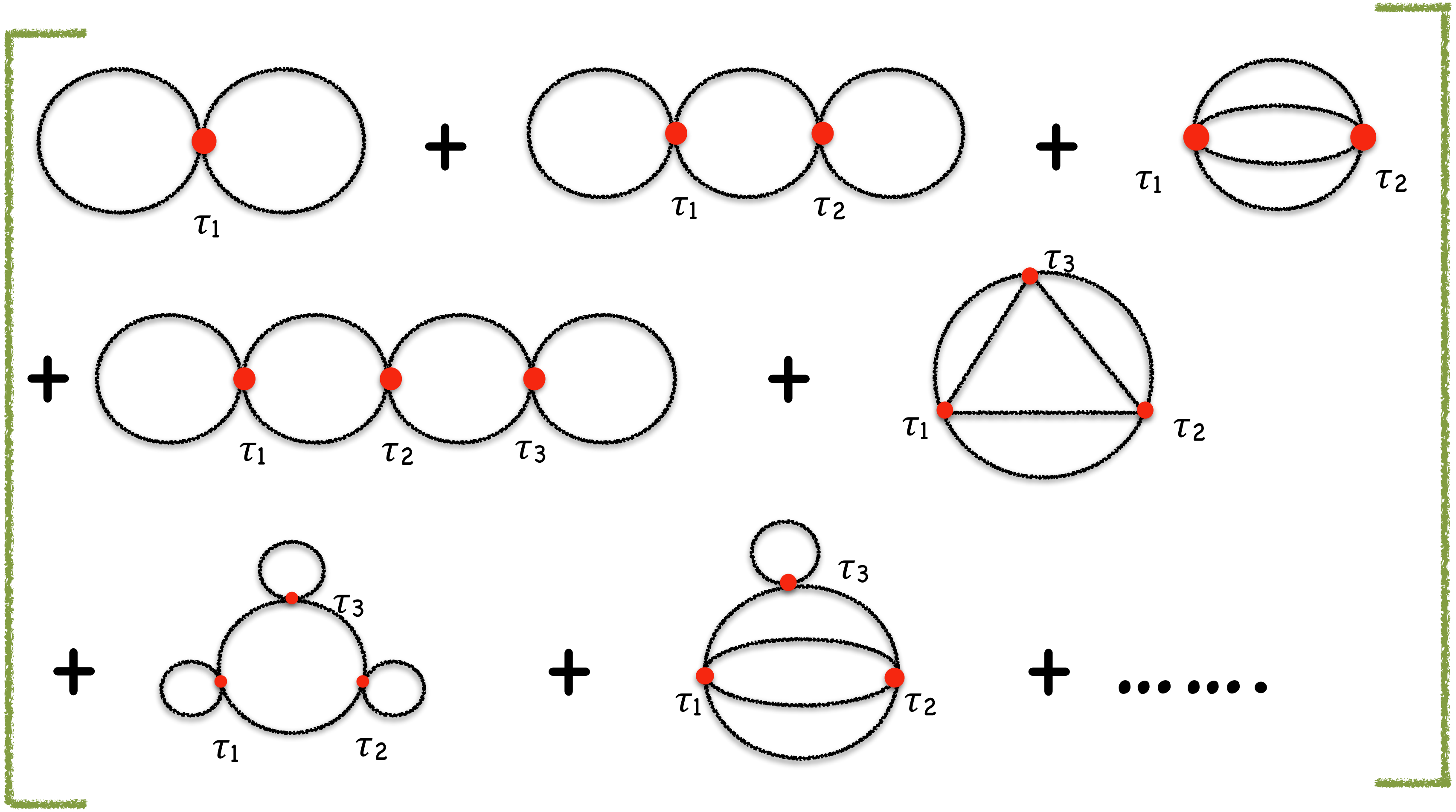
#4) So a diagram with n_c clusters have an addl. symmetry factor of n^{n_c}

Terms linear in n has $n_c = 1$; i.e. only connected clusters contribute to ln Z

Linked Cluster Theorem

Perturbation Theory for Free Energy F

$$-\beta(F - F_0) =$$



How do we evaluate these integrals (diagrams) ?

Since all the integrals involve the 2-pt. function in the Gaussian theory, focus on them

The 2-point function in Gaussian theory

$$\mathcal{G}(\tau_i, \tau_j) = \langle T[x(\tau_i)x(\tau_j)]\rangle_{th} = \frac{\int_{x_0=x}^{x_\beta=x} \mathcal{D}[x(\tau)]x(\tau_i)x(\tau_j)e^{-S_E[x(\tau)]}}{\int_{x_0=x}^{x_\beta=x} \mathcal{D}[x(\tau)]e^{-S_E[x(\tau)]}}$$

For the Harmonic Oscillator $S_E[x(\tau)] = \int_0^\beta d\tau \frac{m}{2}\left[\left(\frac{dx}{d\tau}\right)^2 + \omega_0^2 x^2\right]$

$$\int_0^\beta d\tau \frac{m}{2}\left(\frac{dx}{d\tau}\right)^2 = \frac{m}{2}\frac{dx}{d\tau}x(\tau)\Big|_0^\beta - \frac{m}{2}dx\int_0^\beta d\tau x(\tau)\partial_\tau^2 x(\tau)$$

$$S_E[x(\tau)] = \int_0^\beta d\tau \int_0^\beta d\tau' \frac{m}{2}x(\tau)[-\partial_\tau^2 + \omega_0^2]\delta(\tau-\tau')x(\tau')$$

Time independent system $\mathcal{G}(\tau, \tau') = \mathcal{G}(\tau - \tau')$

Work with the Fourier Transform, G^{-1} is diagonal in that basis

Fourier Transforms in imaginary time formalism

x(τ) is a periodic function with period β (Unlike qnt. fluc. x is not zero at endpoints)

The Fourier transform would involve discrete frequencies $\omega_m = 2\pi m/\beta$ —— m = 0, ±1, ±2, ...

These are called Bosonic Matsubara frequencies

$$x(i\omega_m) = \int_0^\beta d\tau x(\tau) e^{i\omega_m \tau} \qquad x(\tau) = \frac{1}{\beta}\sum_m x(i\omega_m) e^{-i\omega_m \tau}$$

$$\mathcal{G}(\tau - \tau^{'}) \to \mathcal{G}(\tau) = \frac{1}{\beta}\sum_m \mathcal{G}(i\omega_m) e^{-i\omega_m \tau}$$

$$\mathcal{G}(i\omega_m) = \int_0^\beta d\tau \mathcal{G}(\tau) e^{i\omega_m \tau}$$

$$S_E[x(\tau)] = \int_0^\beta d\tau \int_0^\beta d\tau^{'} \frac{m}{2} x(\tau)[-\partial_\tau^2 + \omega_0^2]\delta(\tau - \tau^{'}) x(\tau^{'})$$

$$= \int_0^\beta d\tau \frac{m}{2} x(\tau)[-\partial_\tau^2 + \omega_0^2] x(\tau) \quad = -\frac{m}{2\beta}\sum_m x(i\omega_m)[(i\omega_m)^2 - \omega_0^2] x(-i\omega_m)$$

$$S_E[x(\tau)] = \int_0^\beta d\tau \int_0^\beta d\tau^{'} \frac{1}{2} x(\tau)\mathcal{G}^{-1}(\tau - \tau^{'}) x(\tau^{'})$$

$$= \frac{1}{2}\frac{1}{\beta^3}\int_0^\beta d\tau \int_0^\beta d\tau^{'} \sum_{mnp} x(i\omega_m)\mathcal{G}^{-1}(i\omega_p) x(i\omega_n) e^{-i(\omega_m + \omega_p)\tau} e^{-i(\omega_n - \omega_p)\tau^{'}} = \frac{1}{2}\frac{1}{\beta}\sum_p x(i\omega_p)\mathcal{G}^{-1}(i\omega_p) x(-i\omega_p)$$

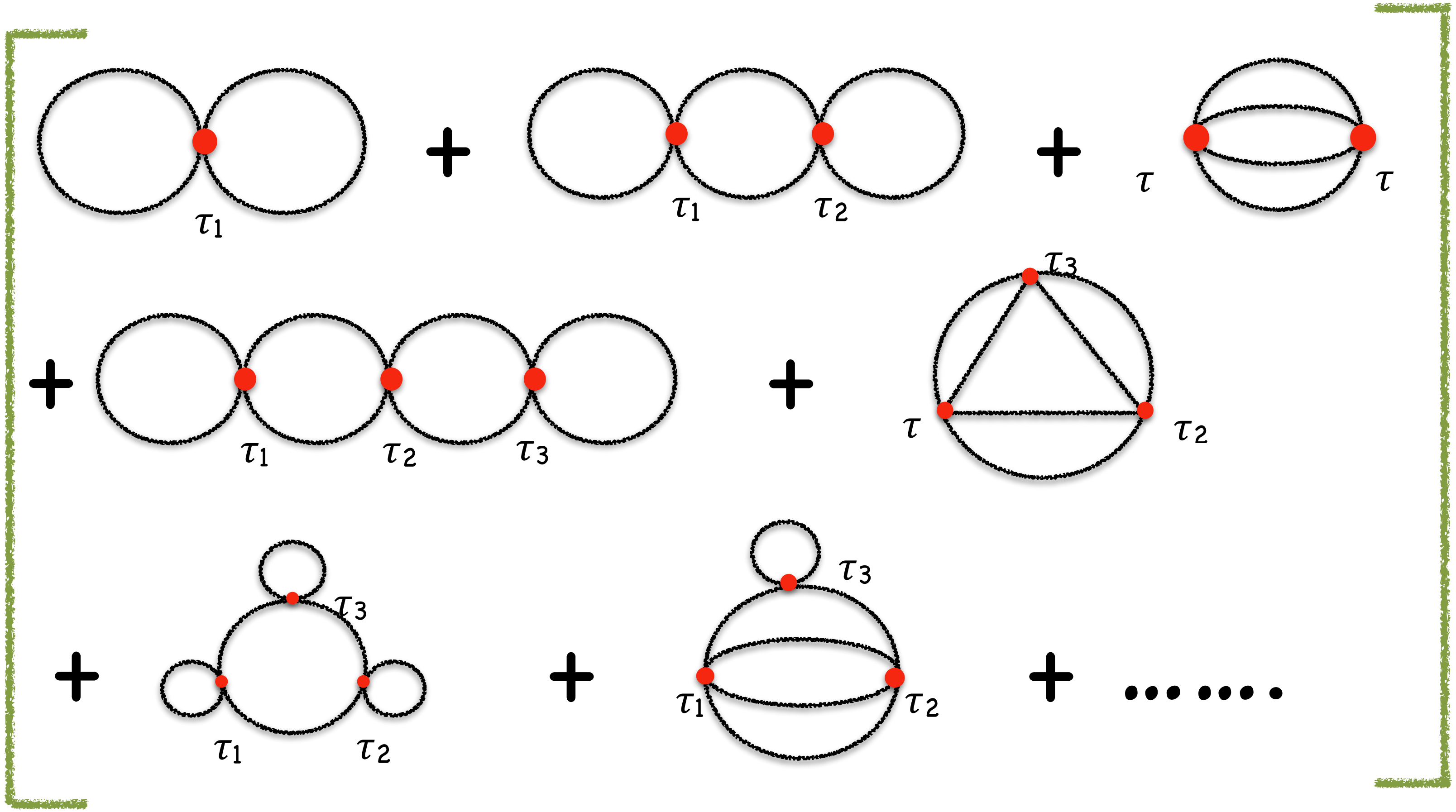
Comparing $\quad \mathcal{G}^{-1}(i\omega_m) = -m[(i\omega_m)^2 - \omega_0^2] \qquad \mathcal{G}(i\omega_m) = -\frac{1}{m}\frac{1}{[(i\omega_m)^2 - \omega_0^2]}$

Perturbative corrections to F

The 2-point fn (in Matsubara frequencies) is given by $\mathcal{G}(i\omega_m) = -\frac{1}{m}\frac{1}{[(i\omega_m)^2 - \omega_0^2]}$

With this knowledge we can now start evaluating the perturbation correction to the Free Energy

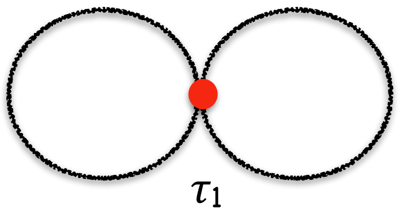
$-\beta(F - F_0) =$



$$Z_0 = \frac{1}{2\sinh[\beta\omega_0/2]} \qquad F_0 = -\frac{1}{\beta}\ln Z_0 = \frac{1}{\beta}\ln(2\sinh[\beta\omega_0/2])$$

Perturbative corrections to F

1st order correction



$$\left(\frac{-1}{\beta}\right)\left(-3\frac{g}{4}\right)\int_0^\beta d\tau_1 \mathcal{G}^2(\tau=0) = \left(\frac{3g}{4}\right)\mathcal{G}^2(\tau=0)$$

$$\mathcal{G}(\tau-\tau^{'}) \to \mathcal{G}(\tau) = \frac{1}{\beta}\sum_m \mathcal{G}(i\omega_m)e^{-i\omega_m \tau}$$

$$\mathcal{G}(0)\frac{1}{\beta}\sum_m \mathcal{G}(i\omega_m) = -\frac{1}{m\beta}\sum_m \frac{1}{(i\omega_m)^2-\omega_0^2}$$

Evaluating Matsubara sums:

The Bose distribution function $n_B(\omega) = \dfrac{1}{e^{\beta\omega}-1}$ has a simple pole at the Matsubara frequencies

$z_0 = i\omega_l = 2\pi\ i\ l/\beta$ —— $l = 0, \pm1, \pm2, \ldots..$

Expanding the denominator near z_0

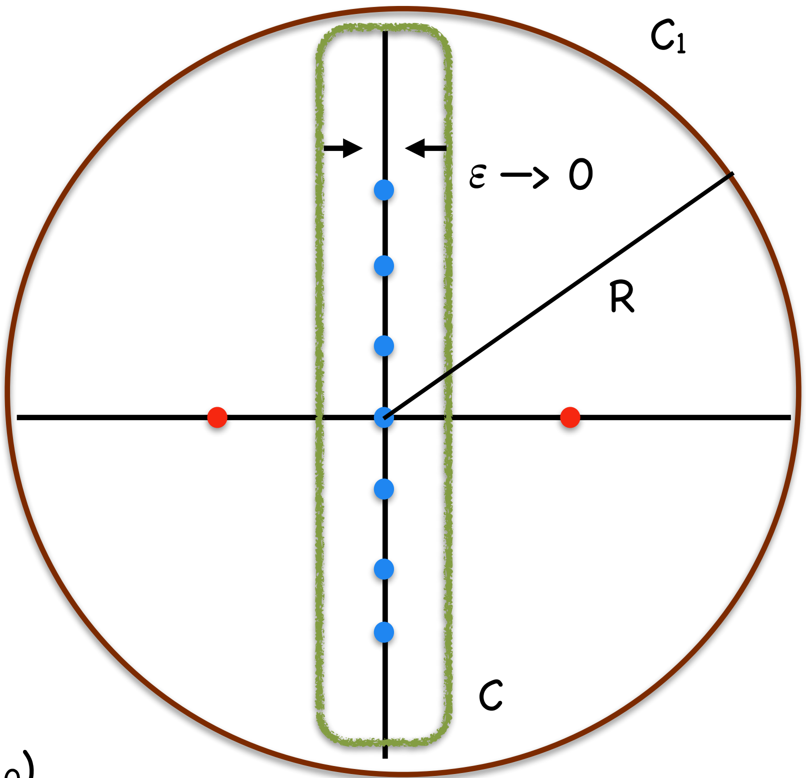
$$e^{\beta z}-1 = e^{\beta z_0}e^{\beta(z-z_0)}-1 = 1+\beta(z-z_0)+\ldots-1 = \beta(z-z_0)+\ldots$$

So the residue at the pole is $1/\beta$

Now Use Cauchy's Residue Theorem in reverse

Perturbative corrections to F

1st order correction



$$\frac{1}{\beta}\sum_l F(i\omega_l) = \oint_C \frac{dz}{2\pi i} n_B(z) F(z)$$

where C is the contour shown, traversed counterclockwise

$$\mathcal{G}(0) = -\frac{1}{m\beta}\sum_m \frac{1}{(i\omega_m)^2 - \omega_0^2} = -\frac{1}{m}\oint_C \frac{dz}{2\pi i} n_B(z) \frac{1}{z^2 - \omega_0^2}$$

$$F(z) = \frac{1}{z^2 - \omega_0^2}$$ has poles at $\pm\ \omega_0$, with residue $\pm 1/(2\omega_0)$

Let us distort the contour C to the contour C_1, which is a circle with radius $R \longrightarrow \infty$

At large R, the integrand ~ $1/R^2$, so the integral on C_1 vanishes

However, in distorting the contour we have added 2 singularities of the fn (the poles), which lie within C_1, but not within C.

$$\mathcal{G}(0) = \frac{1}{m}\sum_{\pm} Res\left[n_B(z)\frac{1}{z^2 - \omega_0^2}\right]\Bigg|_{\pm\omega_0}$$

Perturbative corrections to F

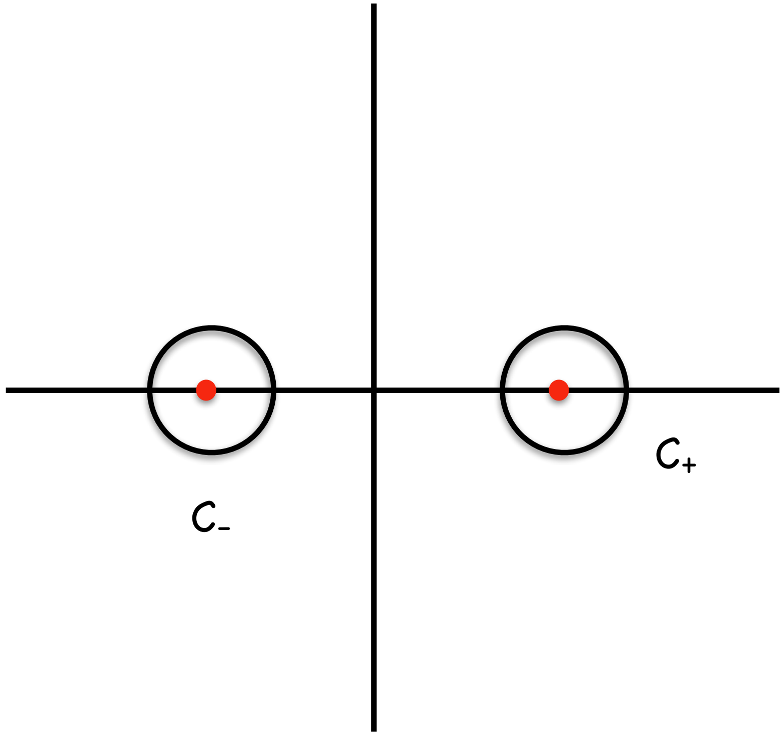
1st order correction

$$\mathcal{G}(0) = \frac{1}{m}\sum_{\pm} Res\left[n_B(z)\frac{1}{z^2-\omega_0^2}\right]\Big|_{\pm\omega_0}$$

$$= \frac{1}{m}\frac{[n_B(\omega_0) - n_B(-\omega_0)]}{2\omega_0}$$

$$= \frac{1}{m}\frac{\coth[\beta\omega_0/2]}{2\omega_0}$$

$$\Delta F^{(1)} = \frac{3g}{4}\left(\frac{1}{m}\frac{\coth[\beta\omega_0/2]}{2\omega_0}\right)^2$$



Going back to real time:

Exponentiate to get $Z^{(1)}/Z_0$

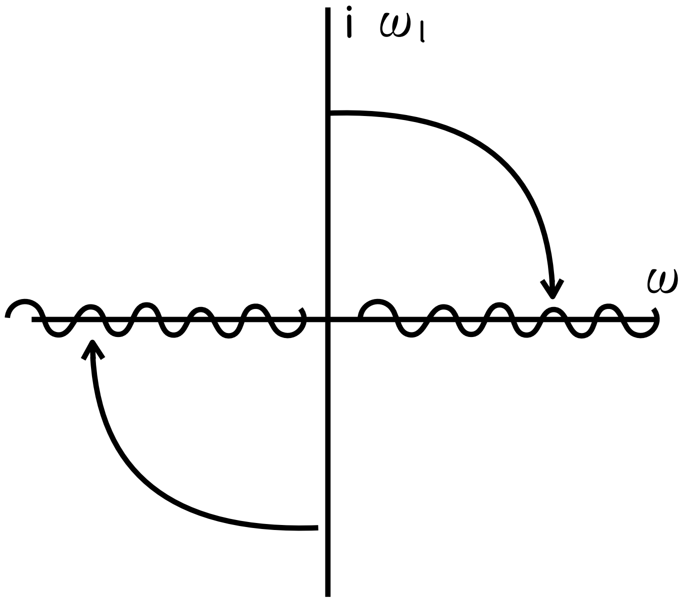
Now use your old dictionary β –> i (t_f–t_i) to go back to real time.

We will leave calculation of 2nd order corrections for HW

Wick Rotation to real Frequencies

We could, alternately, have worked in real time to evaluate the correction (after going to imag. time and using Wick's theorem).

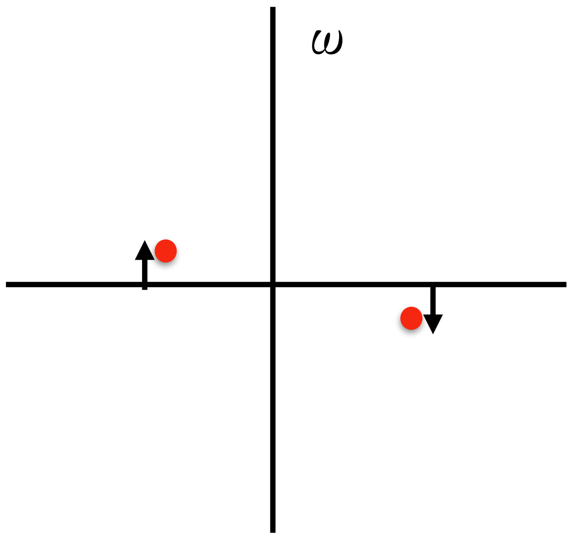
The following rule lets you obtain the time-ordered 2-point function in real frequencies:



$$\mathcal{G}(\omega) = \mathcal{G}[i\omega_l \to \omega + i\eta sgn(\omega)]$$

To get to the real freq, rotate the plane clockwise

The singularities of the 2 pt. fn lies on the real axis. In case of H.O. these are poles. In a more general case this might be branch cuts.



$$\mathcal{G}(i\omega_l) = -\frac{1}{m}\frac{1}{(i\omega_l)^2 - \omega_0^2} = -\frac{1}{2m\omega_0}\left[\frac{1}{i\omega_l - \omega_0} - \frac{1}{i\omega_l + \omega_0}\right]$$

$$\mathcal{G}(\omega) = -\frac{1}{2m\omega_0}\left[\frac{1}{\omega - \omega_0 + i\eta} - \frac{1}{\omega + \omega_0 - i\eta}\right]$$

The poles are shifted to the -ve half-plane for ω > 0 and to +ve half plane for ω<0

Perturbation Expansion for 2-point Fn.s

Suppose we are interested in directly calculating the 2 pt fn for the action with x^4 potential.

Can we develop a perturbation expansion for this quantity directly?

$$\langle T[x(\tau_1)x(\tau_2)]\rangle_{th} = \frac{\left(\frac{m}{2\pi i\epsilon}\right)^{1/2}\int \mathcal{D}[x(\tau)]x(\tau_1)x(\tau_2) \;\; e^{-\int_0^\beta d\tau \frac{m}{2}\dot{x}^2+\frac{m}{2}\omega^2x^2+\frac{g}{4}x^4}}{\left(\frac{m}{2\pi i\epsilon}\right)^{1/2}\int \mathcal{D}[x(\tau)] \;\; e^{-\int_0^\beta d\tau \frac{m}{2}\dot{x}^2+\frac{m}{2}\omega^2x^2+\frac{g}{4}x^4}}$$

$$= \frac{\left(\frac{m}{2\pi i\epsilon}\right)^{1/2}\int \mathcal{D}[x(\tau)]x(\tau_1)x(\tau_2) \;\; e^{-\int_0^\beta d\tau \frac{m}{2}\dot{x}^2+\frac{m}{2}\omega^2x^2+\frac{g}{4}x^4}}{\left(\frac{m}{2\pi i\epsilon}\right)^{1/2}\int \mathcal{D}[x(\tau)] \;\; e^{-\int_0^\beta d\tau \frac{m}{2}\dot{x}^2+\frac{m}{2}\omega^2x^2}} \Bigg/ \frac{\left(\frac{m}{2\pi i\epsilon}\right)^{1/2}\int \mathcal{D}[x(\tau)] \;\; e^{-\int_0^\beta d\tau \frac{m}{2}\dot{x}^2+\frac{m}{2}\omega^2x^2+\frac{g}{4}x^4}}{\left(\frac{m}{2\pi i\epsilon}\right)^{1/2}\int \mathcal{D}[x(\tau)] \;\; e^{-\int_0^\beta d\tau \frac{m}{2}\dot{x}^2+\frac{m}{2}\omega^2x^2}}$$

Let us first work with the numerator

Perturbation Expansion for 2-point Fn.s

$$= \frac{\left(\frac{m}{2\pi i\epsilon}\right)^{1/2} \int \mathcal{D}[x(\tau)] x(\tau_1) x(\tau_2) \quad e^{-\int_0^\beta d\tau \frac{m}{2}\dot{x}^2 + \frac{m}{2}\omega^2 x^2 + \frac{g}{4}x^4}}{\left(\frac{m}{2\pi i\epsilon}\right)^{1/2} \int \mathcal{D}[x(\tau)] \quad e^{-\int_0^\beta d\tau \frac{m}{2}\dot{x}^2 + \frac{m}{2}\omega^2 x^2}}$$

$$G(\tau_1, \tau_2) = \left(\frac{m}{2\pi\epsilon}\right)^{1/2} \int \mathcal{D}[x(\tau)] x(\tau_1) x(\tau_2) \; e^{-\int_0^\beta d\tau \frac{m}{2}\dot{x}^2 + \frac{m}{2}\omega^2 x^2} \left[1 - \frac{g}{4!}\int_0^\beta d\tau' x^4(\tau')\right.$$

$$+ \frac{1}{2!}\left(\frac{g}{4!}\right)^2 \int_0^\beta d\tau' \int_0^\beta d\tau'' x^4(\tau') x^4(\tau'')$$

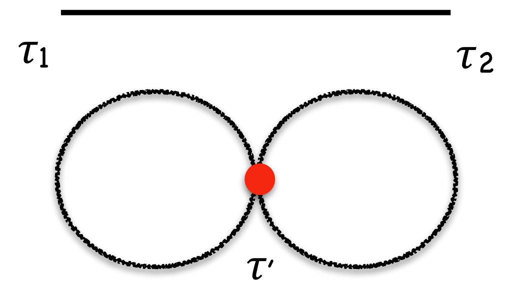
$$+ \ldots\ldots$$

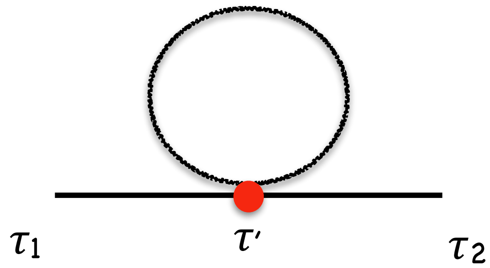
Once again, we can use Wick's theorem to write this term as possible contractions of 2 pt fn.s in the Gaussian Theory.

To keep Track of the terms, we can again use Feynman diagrams

Perturbation Expansion for 2-point Fn.s

Feynman Diagrams upto 1st order





Disconnected Diagram

Connected Diagram

This is G_0 X diagram for Z

cancels with the factor of Z in the denominator

$$-\frac{12g}{4}\int d\tau^{'}\mathcal{G}(\tau_1,\tau^{'})\mathcal{G}(\tau^{'},\tau^{'})\mathcal{G}(\tau^{'},\tau_1)$$

So the thermal expectation value is given by connected correlations, i.e. only connected diagrams contribute. Define interacting 2 pt fn as G and the gaussian 2 pt fn as G_0