# Propagators, Responses, Correlations and Green's Functions

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These notes develop the theories of Green's functions at an elementary level. Section A introduces the method of path integral (sum over all paths) via the propagators for a system of free particles and the harmonic oscillator. In Section B, we give an extra example on using the sum rule method combined with the Green's function to estimate the ground state energy of a 2D harmonic oscillator. Section C is devoted to the density matrix and in Section D we give the first application of using imaginary-time formalism, i.e., simulating the path integral and estimating the ground state energy of a given system. Section E discusses the second example of imaginary-time formalism, namely the thermal effects on a scalar field. Section F introduces the basis of the response functions, correlation functions as well as their inner-connection, the fluctuation–dissipation theorem, here the importance of the retarded response function is emphasized. Section G is on the general theories of (equilibrium) Green's functions, and the spectral function is discussed in some details. In Section H we introduce the concept of spectroscopy which is strongly related to the spectral function, the nucleon momentum distribution in finite nuclei and nuclear matter is also discussed. The last four sections introduce the very basis of non-equilibrium real-time Green's functions (no concept of temperature), their relations with the imaginary-time formalism by analytical continuation, and the closely-related transport equations (conceptual). Exercises and examples are scattered through the notes to help understand the material. A few sections with "∗" could be omitted without influencing the main development (however, certain important concepts do appear in such sections such as the imaginary-time and the Matsubara frequency). [Draft]



## A Propagators: Free Particle and Harmonic Oscillator

Relevant References:

- R. Feynman, *Quantum Mechanics and Path Integrals*, Dover Press, 2010, Chapters 2 and 3.
- A. Zee, *Quantum Field Theory in a Nutshell*, 2nd Edition, Princeton University Press, 2010, Part I.

By using the path integral formulation, one can do relevant quantum mechanical calculations classically. The double-slit experiment tells that the probability amplitude at the detector $D$ is

$$\text{Amplitude}(D) = \sum_{j=1,2} \text{Amplitude}(S \to A_j \to D). \tag{1.1}$$

If there are two walls with one having two slits $A_j$ and the other three slits $B_k$, then the probability amplitude observed at $D$ is

$$\text{Amplitude}(D) = \sum_{j,k} \text{Amplitude}(S \to A_j \to B_k \to D). \tag{1.2}$$

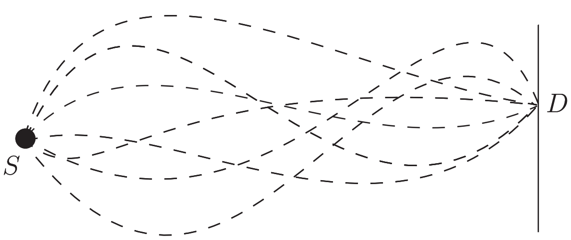


Fig. A: Infinite paths from $S$ to $D$.

A natural question is: If the number of the walls approaches to infinity and in the meanwhile each wall has an infinite number of slits, what is the probability amplitude? In fact, this corresponds to the situation that there is no slits and walls between the source $S$ and the detector $D$, and the probability amplitude is given by

$$\boxed{\text{Amplitude}(D) = \sum_{\text{all paths }(S\to D)} \text{Amplitude}(S \to \cdots \to D),} \tag{1.3}$$

see FIG. A. Our task is to compute the sum of these terms.

Assume that the initial and final coordinates of the system are $q_{\rm i}$ and $q_{\rm f}$, respectively, and the propagation time is

$T$, then the sum of the probability amplitude is given by

$$\langle q_{\rm f}|e^{-iHT/\hbar}|q_{\rm i}\rangle, \tag{1.4}$$

here $\langle q_{\rm f}|e^{-iHT/\hbar}$ represents the time evolution of $\langle q_{\rm f}|$, and when inner-multiplied with $|q_{\rm i}\rangle = |q_{\rm i}\rangle(t=0)$, one obtains the transition probability (propagator or its Green function). Decomposing the time as $\delta = T/N$, then

$$\langle q_{\rm f}|e^{-iHT/\hbar}|q_{\rm i}\rangle = \langle q_{\rm f}|\underbrace{e^{-iH\delta t/\hbar}e^{-iH\delta t/\hbar}\cdots e^{-iH\delta t/\hbar}}_{N\text{ times}}|q_{\rm i}\rangle. \tag{1.5}$$

Using the complete relation of the coordinate namely $\int \mathrm{d}q|q\rangle\langle q| = 1$, one can rewrite the probability amplitude as

$$\langle q_{\rm f}|e^{-iHT/\hbar}|q_{\rm i}\rangle = \left(\prod_{j=1}^{N-1}\int \mathrm{d}q_j\right)\langle q_{\rm f}|e^{-iH\delta t/\hbar}|q_{N-1}\rangle\cdots\langle q_2|e^{-iH\delta t/\hbar}|q_1\rangle\langle q_1|e^{-iH\delta t/\hbar}|q_{\rm i}\rangle. \tag{1.6}$$

The task is to compute the scattering element $\langle q_{j+1}|e^{-iH\delta t/\hbar}|q_j\rangle$. For the free particle, the energy is given by $H = p^2/2m$, and the eigenvalue equation for the momentum operator $p$ is $p|p\rangle = p|p\rangle$, with the eigenvector in the coordinate representation given by $\langle p|q\rangle = (2\pi\hbar)^{-1/2}e^{-ipq/\hbar}$. Thus $\langle q|p\rangle = (2\pi\hbar)^{-1/2}e^{ipq/\hbar}$, then according to the complete relation $\int \mathrm{d}p|p\rangle\langle p| = 1$, one obtains,

$$\langle q_{j+1}|e^{-iH\delta t/\hbar}|q_j\rangle = \int \mathrm{d}p\langle q_{j+1}|\exp\left(-\frac{ip^2\delta t}{2m\hbar}\right)|p\rangle\langle p|q_j\rangle = \frac{1}{2\pi\hbar}\sqrt{\frac{-i2\pi m\hbar}{\delta t}}\exp\left[\frac{i\delta t m}{2\hbar}\left(\frac{q_{j+1}-q_j}{\delta t}\right)^2\right]. \tag{1.7}$$

Multiplying all these elements gives

$$\langle q_{\rm f}|e^{-iHT/\hbar}|q_{\rm i}\rangle = \left(\frac{m}{2\pi\hbar i\delta t}\right)^{N/2}\times\prod_{j=1}^{N-1}\int \mathrm{d}q_j\exp\left[\frac{im\delta t}{2\hbar}\sum_{j=1}^{N-1}\left(\frac{q_{j+1}-q_j}{\delta t}\right)^2\right], \tag{1.8}$$

where $q_0 = q_{\rm i}, q_N = q_{\rm f}$. Since,

$$\left[\frac{q_{j+1}-q_j}{\delta t}\right]^2 \to \dot{q}^2,\quad \sum_{j=1}^{N-1}\to\int_0^T \mathrm{d}t,\quad \int \mathcal{D}q = \lim_{N\to\infty}\left(\frac{m}{2\pi\hbar i\delta t}\right)^{N/2}\prod_{j=1}^{N-1}\int \mathrm{d}q_j, \tag{1.9}$$

we can rewrite the amplitude in the form,

$$\boxed{\langle q_{\rm f}|e^{-iHT/\hbar}|q_{\rm i}\rangle = \int \mathcal{D}q\exp\left(\frac{i}{\hbar}\int_0^T \mathrm{d}t\frac{1}{2}m\dot{q}^2\right),} \tag{1.10}$$

which is the path integral representation of the amplitude for free particle. For system with potential(s), the path integral is generalized to

$$\boxed{\langle q_{\rm f}|e^{-iHT/\hbar}|q_{\rm i}\rangle = \int \mathcal{D}q\exp\left[\frac{i}{\hbar}\int_0^T \mathrm{d}t\left[\frac{1}{2}m\dot{q}^2 - U(q)\right]\right].} \tag{1.11}$$

**EXERCISE 1**: Finish the Gaussian integration in (1.7).
**EXERCISE 2**: Prove the relation (1.11).
**EXERCISE 3**: Derive the classical action for harmonic oscillator.

Slightly rewriting (1.10), one obtains the amplitude for free particle as

$$\boxed{\langle q_{\rm f}|e^{-iHT/\hbar}|q_{\rm i}\rangle = \sqrt{\frac{m}{2\pi\hbar iT}}\times\exp\left[\frac{i}{\hbar}\frac{m(q_{\rm f}-q_{\rm i})^2}{2T}\right].} \tag{1.12}$$

The quantity appearing in the exponential is the classical action $iS_{\rm cl}/\hbar$ with $S_{\rm cl} = \int_{t_1}^{t_2} L(q,\dot{q},t)\mathrm{d}t$. Consider a quadratic Lagrange function, $L(t,q,\dot{q}) = \alpha(t)\dot{q}^2(t)+\beta(t)q(t)\dot{q}(t)+\gamma(t)q^2(t)+\delta(t)\dot{q}(t)+\chi(t)q(t)+\varphi(t)$, where $\alpha(t) = m(t)/2$ is positive. In order to use path integral to deal with the quadratic Lagrange function, one could treat the integration path is formed by fluctuations around the classical path $q_{\rm cl}(t)$ determined by the Lagrange equation. Let $\delta q(t)$ be the perturbation around the classical path, and is called the quantum fluctuation about the classical path. Furthermore, the values of $q(t)$ at the two boundaries $t_{\rm i}, t_{\rm f}$ are fixed and denoted as $q_{\rm i}, q_{\rm f}$. If the quantum fluctuation is not strong enough, the action could be decomposed into two parts, namely the classical action $S[q_{\rm cl}(t)]$ and the quadratic fluctuation part $S_{\rm f}[\delta q(t)]$. Keeping terms up to second order, and considering the equation for $q_{\rm cl}(t)$, we have

$$S[q(t)] = \underbrace{\int_{t_{\rm i}}^{t_{\rm f}} {\rm d}t L(t, q_{\rm cl}, \dot{q}_{\rm cl})}_{S[q_{\rm cl}(t)]} + S_{\rm f}[\delta q(t)], \tag{1.13}$$

where the fluctuation part is given by

$$S_{\rm f}[\delta q(t)] = \int_{t_{\rm i}}^{t_{\rm f}} {\rm d}t \left[\alpha(t)\delta\dot{q}^2 + \beta(t)\delta q\delta\dot{q} + \gamma(t)\delta q^2\right]. \tag{1.14}$$

We call (1.14) the fluctuating action, which is originated from the fluctuation about the classical path, see Fig. B. The above approximation is called the stationary-phase scheme. Under the stationary-phase approximation, then

$$iG(q_{\rm f}, t_{\rm f}; q_{\rm i}, t_{\rm i}) = \langle q_{\rm f}|e^{-iH(t_{\rm f}-t_{\rm i})/\hbar}|q_{\rm i}\rangle = \int \mathcal{D}q(t)e^{iS[q(t)]/\hbar} = \mathscr{F}(t_{\rm f}, t_{\rm i})e^{iS_{\rm cl}/\hbar}, \tag{1.15}$$

$$\mathscr{F}(t_{\rm f}, t_{\rm i}) = \int \mathcal{D}[\delta q(t)] \times \exp\left[\frac{i}{\hbar}\int_{t_{\rm i}}^{t_{\rm f}} {\rm d}t \left[\alpha(t)\delta\dot{q}^2 + \beta(t)\delta q\delta\dot{q} + \gamma(t)\delta q^2\right]\right]. \tag{1.16}$$

Here, $\mathscr{F}(t_{\rm f}, t_{\rm i})$ is the quantum fluctuation factor. If the system is time-translational invariant, the quantum fluctuation factor could be simplified as $\mathscr{F}(t_{\rm f}, t_{\rm i}) = \mathscr{F}(t_{\rm f} - t_{\rm i}) = \mathscr{F}(T)$. The calculation of the quantum fluctuation is extremely important. It also should be pointed out if there exist higher order terms in coordinates or velocities, the stationary-phase approximation will essentially break down.

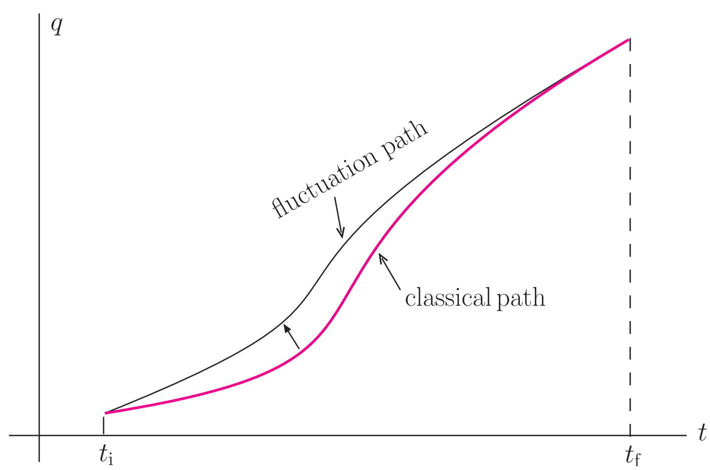


Fig. B: Fluctuation around the classical path.

**EXERCISE 4**: When the stationary-phase approximation breaks down, we should consider high order corrections to the propagator. Prove the following relation:

$$\int e^{n\phi(x)}{\rm d}x \approx e^{n\phi_{\rm max}}\sqrt{\frac{2\pi}{n|\phi''_{\rm max}|}} \times \left[1 + \frac{1}{24n}\left(\frac{3\phi''''_{\rm max}}{\phi''^{,2}_{\rm max}} + \frac{5\phi'''^{,2}_{\rm max}}{\phi''^{,3}_{\rm max}}\right) + \mathcal{O}\left(\frac{1}{n^2}\right)\right]. \tag{1.17}$$

The propagator is then given by in this case (where $\mathcal{N}$ is a constant),

$$iG(q_{\rm f}, t_{\rm f}; q_{\rm i}, t_{\rm i}) \approx \mathcal{N}e^{iS_{\rm cl}/\hbar} \Big/ \det\left(\frac{1}{\hbar}\frac{\delta^2 S[q_{\rm cl}(t)]}{\delta q_{\rm cl}(t)\delta q_{\rm cl}(t')}\right) \times [1 + \mathcal{O}(\hbar)]. \tag{1.18}$$

As an example, we calculate the path integral for the harmonic oscillator in details. The Lagrange function of the harmonic oscillator is given by $L = 2^{-1}m\dot{q}^2 - 2^{-1}m\omega q^2$. The quantum fluctuation is then,

$$\begin{aligned}\mathscr{F}(t_{\rm f} - t_{\rm i}) &= \int \mathcal{D}[\delta q(t)]\exp\left[\frac{i}{2\hbar}\int_{t_{\rm i}}^{t_{\rm f}} {\rm d}t\left(m\delta\dot{q}\delta\dot{q} - m\omega^2\delta q\delta q\right)\right] \\ &= \lim_{N\to\infty}\left(\frac{m}{2\pi i\hbar\delta t}\right)^{N/2}\prod_{j=1}^{N-1}\int {\rm d}\delta q_j \exp\left\{\frac{i\delta t m}{2\hbar}\sum_{j=1}^{N}\left[\left(\frac{\delta q_j - \delta q_{j-1}}{\delta t^2}\right)^2 - \frac{\omega^2(\delta q_j + \delta q_{j-1})^2}{4}\right]\right\}.\end{aligned} \tag{1.19}$$

According to the boundary condition $\delta q(t_\mathrm{i}) = 0 = \delta q(t_\mathrm{f})$, we can set $\delta q_0 = \delta q_N = 0$. By denoting $Q_j = [m/2\hbar\delta t]^{1/2}\delta q_j$,

$$\mathscr{F}(t_\mathrm{f}-t_\mathrm{i}) = \lim_{N\to\infty}\left(\frac{m}{2\pi i\hbar\delta t}\right)^{N/2}\left(\frac{2\hbar\delta t}{m}\right)^{(N-1)/2}\int \mathrm{d}\mathbf{Q}\exp\left(i\mathbf{Q}^\mathrm{T}\vec{\Phi}\mathbf{Q}\right), \tag{1.20}$$

where $\mathbf{Q} = (Q_1,\cdots,Q_{N-1})^\mathrm{T}$. The integration could be done by standard transformation method, and the result is

$$\int \mathrm{d}\mathbf{Q}\exp\left(i\mathbf{Q}^\mathrm{T}\vec{\Phi}\mathbf{Q}\right) = \frac{(i\pi)^{(N-1)/2}}{\sqrt{\det\vec{\Phi}}}. \tag{1.21}$$

The next task is to calculate $\det\vec{\Phi}$. After a long and straightforward derivation, we have

$$\delta t\det\vec{\Phi} = \lim_{N\to\infty}\delta t\det\vec{\Phi}_N = \frac{\sin\omega(t_\mathrm{f}-t_\mathrm{i})}{\omega}, \tag{1.22}$$

leading to the quantum fluctuation as

$$\boxed{\mathscr{F}(t_\mathrm{f}-t_\mathrm{i}) = \left(\frac{m\omega}{2\pi i\hbar\sin\omega(t_\mathrm{f}-t_\mathrm{i})}\right)^{1/2}.} \tag{1.23}$$

On the other hand, the classical action of the oscillator is not hard to calculate,

$$\boxed{S[q_\mathrm{cl}(t)] = \frac{m}{2}\frac{\omega}{\sin\omega(t_\mathrm{f}-t_\mathrm{i})}\left[(q_\mathrm{f}^2+q_\mathrm{i}^2)\cos\omega(t_\mathrm{f}-t_\mathrm{i}) - 2q_\mathrm{f}q_\mathrm{i}\right],} \tag{1.24}$$

see **EXERCISE 3**. Combining the quantum fluctuation and the classical action gives the final expression for the propagator for the harmonic oscillator,

$$\boxed{\langle q_\mathrm{f}|e^{-iH(t_\mathrm{f}-t_\mathrm{i})/\hbar}|q_\mathrm{i}\rangle = \left(\frac{m\omega}{2\pi i\hbar\sin\omega(t_\mathrm{f}-t_\mathrm{i})}\right)^{1/2}\times\exp\left[\frac{i}{\hbar}\frac{m\omega}{2\sin\omega(t_\mathrm{f}-t_\mathrm{i})}\left[(q_\mathrm{f}^2+q_\mathrm{i}^2)\cos\omega(t_\mathrm{f}-t_\mathrm{i}) - 2q_\mathrm{f}q_\mathrm{i}\right]\right].} \tag{1.25}$$

Since the harmonic oscillator is time-translation invariant, we could rewrite the above expression as

$$\boxed{iG = \langle q_\mathrm{f}|e^{-iHT/\hbar}|q_\mathrm{i}\rangle = \left(\frac{m\omega}{2\pi i\hbar\sin\omega T}\right)^{1/2}\times\exp\left[\frac{i}{\hbar}\frac{m\omega}{2\sin\omega T}\left[(q_\mathrm{f}^2+q_\mathrm{i}^2)\cos\omega T - 2q_\mathrm{f}q_\mathrm{i}\right]\right].} \tag{1.26}$$

The limit of this with $\omega\to 0$ is the corresponding propagator for free particles. In fact the propagator for the oscillator can also include an overall phase factor $e^{i\phi(t)}$, where $\phi(t)$ is a function of time.

**EXERCISE 5**: Show that the limit $\omega\to 0$ corresponds to the free case.
**EXERCISE 6**: Prove the identity (1.22).

Based on the result (1.26), one could calculate several relevant quantities for harmonic oscillator. The propagator has the boundary condition $iG(q_\mathrm{f},T;q_\mathrm{i},T) = \delta(q_\mathrm{f}-q_\mathrm{i})$. By calculating the trace of the propagator, we have

$$\begin{aligned}
\int \mathrm{d}q\, iG(q,T;q,0) \equiv \mathrm{tr}\left(e^{-iHT/\hbar}\right) &= \left(\frac{m\omega}{2\pi i\hbar\sin\omega T}\right)^{1/2}\int \mathrm{d}q\exp\left[\frac{i}{\hbar}\frac{m\omega[\cos\omega T-1]q^2}{\sin\omega T}\right]\\
&= \left(\frac{m\omega}{2\pi i\hbar\sin\omega T}\right)^{1/2}\left(\frac{i\pi\hbar\sin\omega T}{m\omega[\cos\omega T-1]}\right)^{1/2} = \frac{1}{2i\sin(\omega T/2)}\\
&= \frac{1}{e^{i\omega T/2}-e^{-i\omega T/2}} = \frac{e^{-i\omega T/2}}{1-e^{-i\omega T}} = \sum_{n=0}^{\infty}\exp\left[-i\left(n+\frac{1}{2}\right)\omega T\right],
\end{aligned} \tag{1.27}$$

from which one immediately obtains the energy level of the oscillator,

$$\boxed{E_n = \left(n+\frac{1}{2}\right)\hbar\omega.} \tag{1.28}$$

Inserting the identity matrix **1** gives the propagator in the following form (in the energy representation)

$$\boxed{iG(q_\mathrm{f},t_\mathrm{f};q_\mathrm{i},t_\mathrm{i}) = \sum_n e^{-(i/\hbar)E_n(t_\mathrm{f}-t_\mathrm{i})}\phi_n(q_\mathrm{f})\phi_n^*(q_\mathrm{i}).} \tag{1.29}$$

Setting $\tau = e^{-i\omega t}$ leads to $2i\sin\omega t = (1-\tau^2)/\tau, 2\cos\omega t = (1+\tau^2)/\tau$, then

$$\begin{aligned}iG(q,t;Q,0) &= \left(\frac{m\omega}{2\pi i\hbar\sin\omega t}\right)^{1/2}\exp\left[\frac{i}{\hbar}\frac{m\omega[(q^2+Q^2)\cos\omega t-2qQ]}{2\sin\omega t}\right]\\ &= \left(\frac{m\omega}{\pi\hbar}\right)^{1/2}\left(\frac{1-\tau^2}{\tau}\right)^{-1/2}\times\exp\left[-\frac{m\omega}{\hbar}\frac{\tau}{1-\tau^2}\frac{(q^2+Q^2)(1+\tau^2)}{2\tau}-2qQ\right]\\ &= \left(\frac{m\omega}{\pi\hbar}\right)^{1/2}\exp\left[-\frac{m\omega(q^2+Q^2)}{2\hbar}\tau^{1/2}(1-\tau^2)^{-1/2}\right]\times\exp\left[\frac{m\omega}{\hbar}\frac{2qQ\tau-(q^2+Q^2)\tau^2}{1-\tau^2}\right].\end{aligned} \tag{1.30}$$

Compare the results with following formula involving Hermite polynomial $H_n(q)$,

$$\sum_{n=0}^{\infty}\frac{(t/2)^n}{n!}H_n(q)H_n(Q) = (1-t^2)^{-1/2}\exp\left(\frac{2qQt-(q^2+Q^2)t^2}{1-t^2}\right), \tag{1.31}$$

the result is

$$iG(q,t;Q,0) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/2}\exp\left(-\frac{m\omega(q^2+Q^2)}{2\hbar}\right)\times\sum_{n=0}^{\infty}\frac{1}{n!2^n}H_n\left(\sqrt{\frac{m\omega}{\hbar}}q\right)H_n\left(\sqrt{\frac{m\omega}{\hbar}}Q\right)\exp\left[-\frac{i}{\hbar}\left(n+\frac{1}{2}\right)\hbar\omega t\right]. \tag{1.32}$$

The wave function for the harmonic oscillator is thus given by

$$\boxed{\phi_n(q) = 2^{-n/2}(n!)^{-1/2}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{m\omega q^2}{2\hbar}\right)H_n\left(\sqrt{\frac{m\omega}{\hbar}}q\right).} \tag{1.33}$$

**EXERCISE 7**: Discuss the classical and quantum probabilities for harmonic oscillator near the equilibrium position.
**EXERCISE 8**: Determine the probability distribution of the various values of the momentum for an oscillator.
**EXERCISE 9**: Find the wave function of the states of a linear oscillator that minimize the uncertainty relation, i.e., which the standard deviation of the coordinate and momentum in the wave packet are related by $\delta p\delta x = \hbar/2$, this is the coherent state.
**EXERCISE 10**: For the forced particle under the constant force $f$, show its path integral for the propagator is given by

$$iG(q_{\rm f},t;q_{\rm i},0) = \left(\frac{m}{2\pi i\hbar t}\right)^{1/2}\times\exp\left[\frac{i}{\hbar}\left[\frac{m(q_{\rm f}-q_{\rm i})^2}{2t}+\frac{1}{2}ft(q_{\rm f}+q_{\rm i})-\frac{f^2t^3}{24m}\right]\right]. \tag{1.34}$$

## B *Green's Function: Sum Rules for a 2D Harmonic Oscillator

RELEVANT REFERENCES:

- The method of QCD sum rules was developed in the following papers: M. Shifman, A. Vainshtein, and V. Zakharov, *QCD and Resonance Physics. Theoretical Foundations*, Nucl. Phys. **B147**, 385 (1979); *ibid*, *QCD and Resonance Physics. Applications*, Nucl. Phys. **B147**, 448 (1979). This section relies on the introductory material from T. Cohen et al., *QCD Sum Rules and Applications to Nuclear Physics*, Prog. Part. Nucl. Phys. **35**, 221 (1995).
- For a full calculation on equation of state of nuclear matter using QCD sum rules is provided in: B.J. Cai and L.W. Chen, *Relativistic Self-energy Decomposition of Nuclear Symmetry Energy and Equation of State of Neutron Matter within QCD Sum Rules*, Phys. Rev. C **100**, 024303 (2019).

The energy level of the 2-dimensional harmonic oscillator is $E_n = (n_x+n_y+1)\hbar\omega = (2n+1)\omega$ (by setting $\hbar = 1$). We develop algorithm to estimate the ground state energy $B \equiv E_0 = \omega$, the method is the sum rule equation.

The Hamiltonian for the two dimensional harmonic oscillator is given by $H(\mathbf{p},\mathbf{q}) = \mathbf{p}^2/2m + 2^{-1}m\omega^2\mathbf{q}^2$, where $\mathbf{p}^2 = p_x^2+p_y^2, \mathbf{q}^2 = x^2+y^2$. The wave function of the ground state is $\phi_0(\mathbf{q}) = (\alpha/\pi)^{1/2}e^{-\alpha\mathbf{q}^2/2}$ with $\alpha = m\omega$ under $\hbar = 1$. At the origin we have $|\phi_0(\mathbf{0})|^2 = m\omega/\pi$, which holds for any order wave functions. The Green's function of the harmonic oscillator is defined as the weighted average of the energy level, i.e.,

$$G(\mathbf{q}_1t_1;\mathbf{q}_2t_2) = \sum_{n=0}^{\infty}\phi_n^*(\mathbf{q}_2)\phi_n(\mathbf{q}_1)e^{-iE_n(t_2-t_1)}, \tag{2.1}$$

see Eq. (1.29). One main ingredient of all types of sum rule approaches is to weaken the contributions from high excited states. In order to do that in the harmonic oscillator, one can introduce the function,

$$\mathscr{U}(\Omega) = \sum_{n=0}^{\infty}|\phi_n(\mathbf{0})|^2e^{-E_n/\Omega}, \tag{2.2}$$

where $\Omega$ is a constant larger than all $E_n$'s, then at the limit $\Omega \to \infty$, only ground state contributes to to $\mathscr{U}(\Omega)$. The function $\mathscr{U}$ is related to $G$ through the analytical continuation, i.e., $\mathscr{U}(\Omega) = G(\mathbf{q}_1 = \mathbf{0}, t_1 = 0; \mathbf{q}_2 = \mathbf{0}, t_2 = 1/i\Omega)$, thus $\Omega$ can be treated as the imaginary time. We have many opportunities to discuss the imaginary time in the following sections. For the harmonic oscillator, we have

$$\mathscr{U}_{\mathrm{osci}}(\Omega) = \sum_n^\infty \frac{m\omega}{\pi} e^{-(2n+1)\omega/\Omega} = \frac{m\omega}{2\pi \sinh(\omega/\Omega)}. \tag{2.3}$$

In the large $\Omega$ limit,

$$\mathscr{U}_{\mathrm{osci}} \approx \frac{m\Omega}{2\pi} \times \left[1 - \frac{1}{6}\left(\frac{\omega}{\Omega}\right)^2 + \frac{7}{360}\left(\frac{\omega}{\Omega}\right)^4 - \frac{31}{15120}\left(\frac{\omega}{\Omega}\right)^6 + \cdots\right]. \tag{2.4}$$

The first term in this expression is the corresponding $\mathscr{U}$ for a free particle, i.e., $\mathscr{U}_{\mathrm{free}}(\Omega) = m\Omega/2\pi$. The terms in the parentheses in Eq. (2.4) are high order corrections originated from the small quantity $\omega/\Omega$. On the other hand, the function $\mathscr{U}_{\mathrm{free}}(\Omega)$ can be written as the sum of energy level of the free particle,

$$\mathscr{U}_{\mathrm{free}}(\Omega) = \int \frac{\mathrm{d}^2\mathbf{k}}{(2\pi)^2} e^{-E_{\mathbf{k}}/\Omega} = \frac{m}{2\pi}\int_0^\infty e^{-E/\Omega}\mathrm{d}E = \frac{1}{\pi}\int_{-\infty}^\infty e^{-E/\Omega}\rho_{\mathrm{free}}(E)\mathrm{d}E, \tag{2.5}$$

where $E_{\mathbf{k}} = \mathbf{k}^2/2m$ is the free particle energy, and $\rho_{\mathrm{free}} = 2^{-1}m\Theta(E)$ is the corresponding density of the energy level, $\Theta$ is the standard step function.

Similarly, the density of the energy level of the oscillator could be given by $\rho_{\mathrm{osci}}(E) = m\omega\sum_{n=0}^\infty \delta(E - (2n+1)\omega)$. Then a series of results can be obtained

$$\boxed{\begin{aligned} \frac{1}{m}\int_0^{2\omega}[\rho_{\mathrm{free}}(E) - \rho_{\mathrm{osci}}(E)]\mathrm{d}E &= 0, && (2.6)\\ \frac{1}{m}\int_{2n\omega}^{(2n+1)\omega}[\rho_{\mathrm{free}}(E) - \rho_{\mathrm{osci}}(E)]\mathrm{d}E &= 0, && (2.7)\\ \frac{1}{m}\int_{2n\omega}^{(2n+1)\omega}[\rho_{\mathrm{free}}(E) - \rho_{\mathrm{osci}}(E)]E\,\mathrm{d}E &= 0, && (2.8)\end{aligned}}$$

etc., which are called dual relations between the free particle and the oscillator. Furthermore,

$$\boxed{\frac{1}{\pi}\int_0^\infty[\rho_{\mathrm{osci}}(E) - \rho_{\mathrm{free}}(E)]e^{-E/\Omega}\mathrm{d}E = \sum_{n=1}\frac{A_n}{\Omega^n},} \tag{2.9}$$

the right hand side of which are the high order effects, which should become smaller and smaller as $\Omega$ increases. It is also obvious that

$$\boxed{\frac{1}{\pi}\int_0^\infty[\rho_{\mathrm{osci}}(E) - \rho_{\mathrm{free}}(E)]\mathrm{d}E = 0,} \tag{2.10}$$

which is another dual relation.

The dual relations indicate that although the structures of the energy level and the wave functions are very different for the free particle and the oscillator, they share large similarities under integrals. Accordingly, we obtain the sum rule equation for the harmonic oscillator through Eq. (2.2) and Eq. (2.4),

$$|\phi_0(\mathbf{0})|^2 e^{-B/\Omega} + \text{“high states”} = \frac{m\Omega}{2\pi} \times \left[1 - \frac{1}{6}\left(\frac{\omega}{\Omega}\right)^2 + \frac{7}{360}\left(\frac{\omega}{\Omega}\right)^4 - \frac{31}{15120}\left(\frac{\omega}{\Omega}\right)^6 + \cdots\right], \tag{2.11}$$

where different "high states" generate different physical consequences. There are no special considerations to define these "high states", and the only requirement is that when $\Omega$ approaches to infinity, effects of the "high states" approach to zero. For instance, if we model the high states like $(m/\pi)e^{-s/\Omega}$ with $s$ the threshold parameter above which the high states contributions become relevant, we then have

$$|\widetilde{\phi}_0(\mathbf{0})|^2 e^{-B/\Omega} \approx \frac{\Omega}{2}\left(1 - e^{-s/\Omega}\right) - \frac{\omega^2}{12\Omega} + \frac{7}{720}\frac{\omega^4}{\Omega^3} - \frac{31}{30240}\frac{\omega^6}{\Omega^5} \quad |\widetilde{\phi}_0(\mathbf{0})|^2 = (\pi/m)|\phi_0(\mathbf{0})|^2. \tag{2.12}$$

After calculating the derivative of Eq. (2.12) with respect to "$-\Omega^{-1}$", we obtain,

$$|\widetilde{\phi}_0(\mathbf{0})|^2 B e^{-B/\Omega} \approx \frac{\Omega^2}{2} - \frac{\Omega^2}{2}e^{-s/\Omega}\left(1 + \frac{s}{\Omega}\right) - \frac{\omega^2}{12} + \frac{7}{240}\frac{\omega^4}{\Omega^2} - \frac{31}{6048}\frac{\omega^6}{\Omega^4}. \tag{2.13}$$

Dividing Eq. (2.12) by Eq. (2.13) gives the formula for the ground state energy $B$,

$$\boxed{B/\omega \approx \frac{1-(1+\nu)e^{-\nu}+1/12-7/240\mathrm{x}^2+31/6048\mathrm{x}^4}{1-e^{-\nu}-1/12\mathrm{x}+7/720\mathrm{x}^3-31/30240\mathrm{x}^5}}, \tag{2.14}$$

with $\mathrm{x}=\Omega/\omega, f=s/\omega, \nu=f/\mathrm{x}$, this is the sum rule equation for the harmonic oscillator in two dimensions. Several ingredients related to the above method are necessary to be pointed out:

(a) The result for $B$ depends on the approximation of the high states, and in the above example, the approximation is modeled as $e^{-s/\Omega}$.

(b) For a fixed approximation for the high states, the result for $B$ depends on $s$ and $\Omega$. One hopes that at a certain range of $\Omega$, the result for $B$ is insensitive to $\Omega$. This range is often called the smooth region (window) which is of course related to the value of $s$ (or $f$).

(c) If the approximation for the high states is selected unreasonable, there may not exist the smooth region.

If Eq. (2.12) is truncated, e.g., at order $\omega^2$, one then obtains

$$\boxed{B/\omega \approx \frac{1-(1+\nu)e^{-\nu}+1/12}{1-e^{-\nu}-1/12\mathrm{x}}}. \tag{2.15}$$

From either Eq. (2.15) or Eq. (2.14), we have approximately $B/\omega \approx 1$.

**EXERCISE 11**: Estimate the ground state energy $B$ using Eq. (2.14) and (2.15) and do the sensitive analysis.
**EXERCISE 12**: Adopt the "high states" via $\exp[-(s/\Omega)^n]$, do the similar sum rule calculations.

**Comments.** This very simple example on estimating the ground state energy of the 2D harmonic oscillator shares many similarities of the sum rule (SR) equations used in quantum chromodynamics (QCD): (a) The $\Omega$ in the sum rule equations for the harmonic oscillator is very similar as the Borel mass $\mathscr{M}$ in QCDSR, e.g., the smooth region (QCDSR window) of $\mathscr{M}^2$ is found to be about $0.8\,\mathrm{GeV}^2 \lesssim \mathscr{M}^2 \lesssim 1.4\,\mathrm{GeV}^2$; (b) Similarly in QCDSR, the nucleon correlation functions should be constructed by the Lorentz structure of the nucleon self-energies, and they also contain relevant information on the high states effects. Moreover, the high states effects on the physical quantities are weakened (even to be removed) by the Borel transformation, which plays a central role in QCDSR; (c) On the other hand, quark/gluon correlation functions (or more precisely, the quark/gluon condensates) are constructed via the operator product expansion (OPE) method, which is similar to the expansion of the weighted average sum of energy level, i.e., $\mathscr{U}_{\mathrm{osci}}$, on the small parameter $\omega/\Omega$. The OPE coefficients, called Wilson's coefficients, are determined by standard perturbative methods in quantum field theories; and (d) in QCDSR, the quark/gluon condensates such as $\langle\overline{q}q\rangle$ and $\langle G^2\rangle$ with $q$ and $G$ the quark and gluon fields are determined by experimental analysis or microscopic calculations.

## C Density Matrix (Elementary Introduction)

RELEVANT REFERENCE:

- R. Feynman, *Statistical Mechanics: a Set of Lectures*, CRC Press, 1998, Chapter 2.

Density matrix is the straightforward generalization of the wave function. Consider an ensemble consisting of $N$ systems, where $N \gg 1$. The state of the system is characterized by the vector $|K\rangle, K=1,2,\cdots,N$. By introducing the orthogonal and normalized basis $|n\rangle$ and writing the state in terms of the basis as $|K\rangle=\sum_n\langle n|K\rangle|n\rangle$, one finds that $\langle n|K\rangle$ is the wave function in the representation of the basis $|n\rangle$, according to the principle of quantum mechanics. An average of the quantity $f$ on the $K$th system is thus calculated as $f_K=\langle K|f|K\rangle$, and the ensemble expectation over $f_K$ is

$$\boxed{\langle f\rangle=\frac{1}{N}\sum_{K=1}^{N}\langle K|f|K\rangle=\frac{1}{N}\sum_{K=1}^{N}\sum_{m,n}\langle K|m\rangle\langle m|f|n\rangle\langle n|K\rangle}, \tag{3.1}$$

where $\langle m|f|n\rangle$ is the matrix element of the operator $f$ in the $n$-representation. Let's define the matrix element of the density matrix $\rho$ as $\rho_{mn}=\sum_K\langle m|K\rangle\langle K|n\rangle/N$, and thus $\langle f\rangle=\sum_{m,n}f_{mn}\rho_{nm}=\mathrm{tr}(\rho f)$. In quantum statistical problems, the ensemble average of any quantity could be expressed as the trace of the product between the operator and the density matrix, and this is the quadratic average namely both quantum-mechanically and statistically. If one writes the density matrix in the form independent of the representation used, then $\rho=\sum_K|K\rangle\langle K|/N$. A few properties of the density matrix:

(a) The density matrix is Hermitian, i.e., $\rho_{mn}=\rho_{nm}^*$.

(b) The trace is 1, and the diagonal elements are non-negative, i.e., $\sum_n\rho_{nn}=1, 0\le\rho_{nn}\le1$.

Selecting the representation in which the density matrix is diagonal, i.e., $\rho_{mn} = \rho_m \delta_{mn}$. Since,

$$\operatorname{tr}\left(\rho^2\right) = \sum_m \rho_m^2 \le \left(\sum_m \rho_m\right)^2 = 1, \tag{3.2}$$

and the trace of a matrix is invariant under the unitary transform, thus the $\rho$ in the non-diagonal representation,

$$\sum_{n,m} \rho_{mn}\rho_{nm} = \sum_{m,n} |\rho_{mn}|^2 \le 1, \tag{3.3}$$

which puts constraints on each element of the density matrix. The diagonal element could be written explicitly as

$$\rho_{nn} = \frac{1}{N}\sum_K \langle n|K\rangle\langle K|n\rangle = \frac{1}{N}\sum_K |\langle n|K\rangle|^2. \tag{3.4}$$

According to quantum mechanics, $|\langle n|K\rangle|^2$ is the probability of the $K$th system on the state $|n\rangle$, and averagely the probability of any system of the ensemble on the state $|n\rangle$ is $\rho_{nn}$. In this sense, the diagonal element of the density matrix characterizes the probability of the system of the ensemble staying on a certain state, and consequently it is very likely that the density matrix shares the similarity of the probability density in classical physics.

There are two ensembles namely the pure ensemble and the mixed ensemble in quantum statistics. If every system of the ensemble is staying at the same quantum state, we call the ensemble the pure ensemble. In this case, wave function is enough to describe the ensemble, otherwise the ensemble is mixed. Naturally for the pure ensemble, we have $\rho^2 = \rho$, i.e., only one of the diagonal elements of the density matrix is 1 and all the others are zero. In the non-diagonal representation, the pure density corresponds to

$$\rho_{mn} = \frac{1}{N}\sum_{K=1}^{N} \langle m|K\rangle\langle K|n\rangle \equiv \langle m|K\rangle\langle K|n\rangle, \tag{3.5}$$

$$\rho_{mn}^2 = \sum_l \rho_{ml}\rho_{ln} = \sum_l \langle m|K\rangle\langle K|l\rangle\langle l|K\rangle\langle K|n\rangle = \langle m|K\rangle\langle K|n\rangle = \rho_{mn}. \tag{3.6}$$

Let $H$ be the Hamiltonian function of the system, then

$$i\hbar\frac{\partial}{\partial t}\rho = i\hbar\frac{\partial}{\partial t}\left(\frac{1}{N}\sum_K |K\rangle\langle K|\right) = \sum_K \frac{1}{N} H|K\rangle\langle K| - \sum_K \frac{1}{N}|K\rangle\langle K|H = [H,\rho], \tag{3.7}$$

which is called the quantum Liouville's equation. From the quantum Liouville's equation, one can immediately obtain the time evolution of the average of the physical quantity

$$i\hbar\frac{\mathrm{d}\langle f\rangle}{\mathrm{d}t} = \operatorname{tr}\left(i\hbar\frac{\partial\rho}{\partial t}f + i\hbar\rho\frac{\partial f}{\partial t}\right) = \operatorname{tr}\left([H,\rho]f + i\hbar\rho\frac{\partial f}{\partial t}\right) = \operatorname{tr}\left(\rho\left[i\hbar\frac{\partial f}{\partial t} + [f,H]\right]\right) = i\hbar\left\langle\frac{\partial f}{\partial t}\right\rangle + \langle [f,H]\rangle, \tag{3.8}$$

If one knows the density matrix, then all the properties of the physical quantities could be obtained. For a system in equilibrium, we have $\partial\rho/\partial t = 0$, i.e., $[\rho, H] = 0$, indicating that $\rho$ is a function of $H$. In addition, if the Hamiltonian $H$ is time-independent, one can choose the eigenstate of $H$., i.e., $|n\rangle$ to do the calculations, and in this case $\rho_{mn} = \rho_n\delta_{mn}$.

Two frequently-used ensembles are the micro-canonical and the canonical ensembles. In the micro-canonical ensemble, the energy $E$ is fixed, thus $\rho_{mn} = \rho_n\delta_{mn}$, where $\rho_n = W^{-1}$ for $E \le E_K \le E + \delta$. All the thermodynamic properties of the system/ensemble could be determined by the entropy $S = k_{\mathrm{B}} \ln W$. For the pure ensemble, the number of microstates is 1, thus $S = 0$. In the canonical ensemble, the energy $E$ is not fixed, but could change by exchanging with the external system. The density matrix is $\rho_{mn} = \rho_n\delta_{mn}$, where $\rho_n = Z^{-1}e^{-\beta E_n}$, here

$$\boxed{Z = \operatorname{tr}\left(e^{-\beta H}\right) = \sum_n e^{-\beta E_n},} \tag{3.9}$$

is the partition function. Moreover,

$$\rho = \frac{1}{N}\sum_K |K\rangle\langle K| = \frac{1}{N}\sum_{mn}\sum_K |E_m\rangle\langle E_m|K\rangle\langle K|E_n\rangle\langle E_n| = \sum_n \rho_n|E_n\rangle\langle E_n| = \frac{e^{-\beta H}}{Z}\sum_n |E_n\rangle\langle E_n| = \frac{e^{-\beta H}}{\operatorname{tr}(e^{-\beta H})}. \tag{3.10}$$

The average of the physical quantity $f$ in the canonical ensemble is

$$\langle f\rangle = \operatorname{tr}\left(\rho f\right) = \frac{\operatorname{tr}(f e^{-\beta H})}{\operatorname{tr}(e^{-\beta H})} = \frac{\sum_n f_n e^{-\beta E_n}}{\sum_n e^{-\beta E_n}}, \tag{3.11}$$

where $f_n$ is the eigenvalue of the $f$ corresponding to the eigenstate $E_n$. The density matrix in the coordinate representation could be calculated as:

$$\boxed{\rho\left(\mathbf{x}^N,\mathbf{x}^{N'}\right)=\langle\mathbf{x}^N|\rho|\mathbf{x}^{N'}\rangle=\sum_n e^{-\varphi-\beta E_n}\langle\mathbf{x}^N|E_n\rangle\langle E_n|\mathbf{x}^{N'}\rangle=\sum_n e^{-\varphi-\beta E_n}\phi_n(\mathbf{x}^N)\phi_n^*(\mathbf{x}^{N'}),} \tag{3.12}$$

here $\langle\mathbf{x}^N|E_n\rangle\equiv\phi_n(\mathbf{x}^N)$ is the expression for the energy eigenstate in the coordinate representation (with $N$ particles).

**Example – 1.** We calculate the density matrix of the ensemble consisting of free particles. The eigen-function of the free particle with mass $m$ placed in the cube with side length $L$ is given by $\phi_E(\mathbf{x})=L^{-3/2}e^{i\mathbf{k}\cdot\mathbf{x}}$ under the periodic boundary condition, and the eigenvalue is $E=\hbar^2k^2/2m$. The density matrix of the canonical ensemble in the coordinate representation is

$$\langle\mathbf{x}|e^{-\beta H}|\mathbf{x}'\rangle=\sum_E\langle\mathbf{x}|E\rangle e^{-\beta E}\langle E|\mathbf{x}'\rangle=\sum_n e^{-\beta E}\phi_E(\mathbf{x})\phi_E^*(\mathbf{x}')=\frac{1}{L^3}\sum_{\mathbf{k}}\exp\left[-\frac{\beta\hbar^2k^2}{2m}+i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')\right]. \tag{3.13}$$

One can approximate the sum here by integration if the volume $V$ is very large, using $\sum_{\mathbf{k}}\to L^3\int\mathrm{d}\mathbf{k}/(2\pi)^3$,

$$\langle\mathbf{x}|e^{-\beta H}|\mathbf{x}'\rangle=\frac{1}{(2\pi)^3}\int\exp\left[-\frac{\beta\hbar^2k^2}{2m}+i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')\right]\mathrm{d}\mathbf{k}=\left(\frac{m}{2\pi\beta\hbar^2}\right)^{3/2}\exp\left[-\frac{m}{2\beta\hbar^2}(\mathbf{x}-\mathbf{x}')^2\right], \tag{3.14}$$

therefore

$$\boxed{\mathrm{tr}\left(e^{-\beta H}\right)=\int\langle\mathbf{x}|e^{-\beta H}|\mathbf{x}\rangle\mathrm{d}\mathbf{x}=V\left(\frac{m}{2\pi\beta\hbar^2}\right)^{3/2}.} \tag{3.15}$$

This is the partition function of the free particle, from which one can calculate the density matrix as

$$\boxed{\rho(\mathbf{x},\mathbf{x}')=\langle\mathbf{x}|\rho|\mathbf{x}'\rangle=\frac{\langle\mathbf{x}|e^{-\beta H}|\mathbf{x}'\rangle}{\mathrm{tr}(e^{-\beta H})}=\frac{1}{V}\exp\left[-\frac{m}{2\beta\hbar^2}(\mathbf{x}-\mathbf{x}')^2\right].} \tag{3.16}$$

**EXERCISE 13**: Derive the partition function (3.15) using conventional method.

It could be found that the diagonal element of the density matrix is $\rho(\mathbf{x},\mathbf{x})=1/V$, which is independent of the position $\mathbf{x}$, indicating the probability the particle being at any position in the box is the same. Moreover, the off-diagonal element of the density matrix $\rho(\mathbf{x},\mathbf{x}')$ characterizes the spontaneous transition probability between position $\mathbf{x}$ and $\mathbf{x}'$, and this correlation effect is a pure quantum behavior. If the temperature $T$ is high, the above expression approaches to a $\delta$ function, i.e., the system is classical. We can then calculate the average of the Hamiltonian as

$$\begin{aligned}\langle H\rangle=\mathrm{tr}(\rho H)&=\int\mathrm{d}\mathbf{x}\mathrm{d}\mathbf{x}'\langle\mathbf{x}|\rho|\mathbf{x}'\rangle\langle\mathbf{x}'|H|\mathbf{x}\rangle\\&=-\frac{\hbar^2}{2mV}\int\mathrm{d}\mathbf{x}\mathrm{d}\mathbf{x}'\exp\left[-\frac{m}{2\beta\hbar^2}(\mathbf{x}-\mathbf{x}')^2\right]\nabla_{\mathbf{x}}^2\delta(\mathbf{x}-\mathbf{x}')\\&=-\frac{\hbar^2}{2mV}\int\mathrm{d}\mathbf{x}\mathrm{d}\mathbf{x}'\delta(\mathbf{x}-\mathbf{x}')\nabla_{\mathbf{x}}^2\exp\left[-\frac{m}{2\beta\hbar^2}(\mathbf{x}-\mathbf{x}')^2\right]\\&=-\frac{\hbar^2}{2mV}\int\mathrm{d}\mathbf{x}'\left[\nabla_{\mathbf{x}}^2\exp\left[-\frac{m}{2\beta\hbar^2}(\mathbf{x}-\mathbf{x}')^2\right]\right]_{\mathbf{x}=\mathbf{x}'}=\frac{3}{2}k_{\mathrm{B}}T.\end{aligned} \tag{3.17}$$

**Example – 2.** We now calculate the density matrix of the harmonic oscillator. The density matrix takes the form of $\rho=e^{-\beta H}/\mathrm{tr}(e^{-\beta H})$, which could be re-expressed in the energy representation as $\rho_{nm}\sim\delta_{nm}e^{-\beta E_n}$. Taking the derivative with respective to $\beta$ gives $-\partial\rho_{nm}/\partial\beta=\delta_{nm}E_ne^{-\beta E_n}=E_n\rho_{nm}$, which is the same as $-\partial\rho/\partial\beta=H\rho$. This is the Bloch's equation for $\rho$, with the initial condition $\rho(0)=1$. In the coordinate representation, we have

$$\boxed{-\frac{\partial\rho(q,q';\beta)}{\partial\beta}=H\rho(q,q';\beta),\quad\rho(q,q';0)=\delta(q-q').} \tag{3.18}$$

For the harmonic oscillator, the Bloch's equation reads

$$-\frac{\partial\rho}{\partial\beta}=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial q^2}\rho+\frac{1}{2}m\omega^2q^2\rho. \tag{3.19}$$

The solution of it is given by,

$$\boxed{\rho(q,q';\beta)=\left(\frac{m\omega}{2\pi\hbar\sinh\beta\hbar\omega}\right)^{1/2}\times\exp\left[-\frac{m\omega}{2\hbar\sinh\beta\hbar\omega}\left[\left(q^2+q'^2\right)\cosh\beta\hbar\omega-2qq'\right]\right].} \tag{3.20}$$

**EXERCISE 14**: Solve Bloch's equation for the harmonic oscillator by transforming to $\xi=(m\omega/\hbar)^{1/2}q, f=\hbar\omega\beta/2$ and considering the appropriate limit of $f\to 0$.

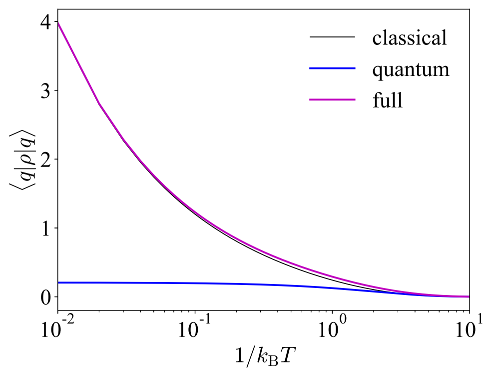


Fig. C: $\langle q|\rho|q\rangle$ as a function of $1/k_{\mathrm{B}}T$.

If one takes $q=q'$ in the above expression, then

$$\rho(q,q;\beta)=\left(\frac{m\omega}{2\pi\hbar\sinh\beta\hbar\omega}\right)^{1/2}\times\exp\left(-\frac{m\omega q^2}{\hbar}\tanh\frac{\beta\hbar\omega}{2}\right), \tag{3.21}$$

thus

$$\mathrm{tr}\left(e^{-\beta H}\right)=\int\rho(q,q;\beta)\mathrm{d}q=\frac{1}{2\sinh(\beta\hbar\omega/2)}=\frac{e^{-\beta\hbar\omega/2}}{1-e^{-\beta\hbar\omega}}, \tag{3.22}$$

which is the partition function for a single oscillator. In addition,

$$\langle q^2\rangle=\int q^2\rho(q,q;\beta)\mathrm{d}q\Big/\int\rho(q,q;\beta)\mathrm{d}q=\frac{\hbar}{2m\omega}\coth\frac{\beta\hbar\omega}{2}, \tag{3.23}$$

and consequently,

$$\langle U\rangle=\frac{1}{2}m\omega^2\langle q^2\rangle=\frac{\hbar\omega}{4}\coth\frac{\beta\hbar\omega}{2}, \tag{3.24}$$

$$\langle K\rangle=\left\langle-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial q^2}\right\rangle=\frac{\hbar\omega}{4}\coth\frac{\beta\hbar\omega}{2}. \tag{3.25}$$

The total energy is

$$\boxed{\langle E\rangle=\langle U\rangle+\langle K\rangle=\frac{\hbar\omega}{2}\coth\frac{\beta\hbar\omega}{2}.} \tag{3.26}$$

**EXERCISE 15**: Discuss the high- and low-temperature limits of the density matrix (3.21).
**EXERCISE 16**: The behavior of a system is either classical or quantum-mechanical is determined by the thermal wavelength,

$$\lambda_{\mathrm{th}}=\sqrt{\frac{h^2}{2\pi mk_{\mathrm{B}}T}}. \tag{3.27}$$

Estimate at which temperature the de Broglie wavelength is comparable to the thermal wavelength.

## D *Imaginary Time $\beta\hbar\leftrightarrow it$, Path Integral Simulations

RELEVANT REFERENCES:

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There exists close connection between the density matrix and the transition probability. For example, for the 1D free particle, the transition amplitude from $q_{\mathrm{i}}$ to $q_{\mathrm{f}}$ is given by

$$\langle q_{\mathrm{f}}|e^{-iHt/\hbar}|q_{\mathrm{i}}\rangle=\left(\frac{m}{2\pi i\hbar t}\right)^{1/2}\exp\left[\frac{i}{\hbar}\frac{m(q_{\mathrm{f}}-q_{\mathrm{i}})^2}{2t}\right], \tag{4.1}$$

see Eq. (1.12). Similarly, the density matrix for the free particle $\langle q_{\mathrm{f}}|e^{-\beta H}|q_{\mathrm{i}}\rangle$ is

$$\langle q_{\mathrm{f}}|e^{-\beta H}|q_{\mathrm{i}}\rangle=\left(\frac{m}{2\pi\beta\hbar^2}\right)^{1/2}\exp\left[-\frac{m(q_{\mathrm{f}}-q_{\mathrm{i}})^2}{2\beta\hbar^2}\right], \tag{4.2}$$

see Eq. (3.16). We can easily find if one uses $\beta\hbar = it$ in Eq. (4.2), then Eq. (4.1) is naturally obtained. This means the density matrix in statistical mechanics can be obtained from the transition probability in quantum mechanics (and vice versa). We often call $\beta = 1/k_{\mathrm{B}}T$ the imaginary time, which fundamentally encapsulates the physics of temperature (therefore it describes equilibrium states.

**EXERCISE 17**: Establish this connection for the harmonic oscillator similarly.

Since the density matrix and the transition probability is strongly related via the imaginary time, one can also formulate the path integral for the density matrix. Since the structures of $\langle q_{\mathrm{f}}|e^{-\beta H}|q_{\mathrm{i}}\rangle$ and $\langle q_{\mathrm{f}}|e^{-iHt/\hbar}|q_{\mathrm{i}}|\rangle$ are very similar, we start from the following probability,

$$\langle q_{\mathrm{f}}|e^{-iH(t_{\mathrm{f}}-t_{\mathrm{i}})/\hbar}|q_{\mathrm{i}}\rangle = \int \mathcal{D}q \exp\left[\frac{i}{\hbar}\int_{t_{\mathrm{i}}}^{t_{\mathrm{f}}}\left[\frac{1}{2}m\dot{q}^2 - U(q)\right]\right], \tag{4.3}$$

here the factor appeared in the exponential is the action. Making $t = -i\tau$(which is also called the Wick's rotation, here we find $\beta\hbar \sim it \sim \tau$) gives

$$iS|_{t=-i\tau} = \int_{\tau_{\mathrm{i}}}^{\tau_{\mathrm{f}}} \mathrm{d}\tau \left[-\frac{m}{2}\left(\frac{\mathrm{d}q}{\mathrm{d}\tau}\right)^2 - U(q)\right] = -S_{\mathrm{E}}. \tag{4.4}$$

After introducing the Euclidean action $S_{\mathrm{E}}$, we transform the factor $e^{iS/\hbar}$ to $e^{-S_{\mathrm{E}}/\hbar}$(sometimes we also write it as $e^{S_{\mathrm{E}}/\hbar}$ which has a sign difference). The partition function is obtained as its path integral representation,

$$\boxed{Z(\beta) = \mathrm{tr}\left(e^{-\beta H}\right) = \int \mathrm{d}q \langle q|e^{-\beta H}|q\rangle = \int_{q(0)=q(\beta)} \mathcal{D}[q(\tau)]\exp\left[-\frac{1}{\hbar}\int_0^{\beta}\mathrm{d}\tau\left[\frac{1}{2}m\dot{q}(\tau) + U(q(\tau))\right]\right],} \tag{4.5}$$

here the measure $\mathcal{D}[q(\tau)]$ contains the product of $N$ terms and $\dot{q}$ represents the derivative with respect to $\tau$. The trace operation sets the initial and final states equal and so the functional integral should be worked out over all paths with the periodic boundary condition $q(0) = q(\beta)$. Eq. (4.5) also tells that the Euclidean quantum field theory in $(d+1)$-dimensional space-time with $0 \le \tau \le \beta$ is equivalent to quantum statistical mechanics in $d$-dimensional space. In order to investigate a field theory at finite temperature all one needs to do is rotate it to Euclidean space and impose the corresponding periodic boundary condition.

The periodic boundary condition $q(0) = q(\beta)$ means only periodic orbits make contribution to the partition function. The path integral formulation of the partition function finds wide applications in field theory problems, like the decay of meta-stable states, the instanton statistical problem, etc. We can use the above idea to do Monte Carlo simulation and find certain properties of the system under consideration. Firstly, we denote $iG$ by $K$ and introduce $\epsilon = i\delta t$, then the propagator for the system under influence $U(q)$ could be written as

$$K(q,q_0;N,\epsilon) = \left(\frac{m}{2\pi\hbar\epsilon}\right)^{N/2}\int \mathrm{d}q_1\cdots\mathrm{d}q_{N-1} \times \exp\left[\frac{\epsilon}{\hbar}\sum_{j=1}^{N}\left[\frac{m}{2}\left(\frac{q_j - q_{j-1}}{\delta t}\right)^2 - U(q_j)\right]\right], \tag{4.6}$$

here $N\epsilon = \tau$ (imaginary time), this is a high-dimensional integration which could be evaluated by efficient Monte Carlo algorithm (e.g., the Metropolis). Next by introducing $\tau = it$ and $t_0 = 0$, we can write the propagator $K(q,\tau;q,0)$ as $K(q,\tau;q,0) = \sum_n \phi_n(q)\phi_0(q_0)e^{-\tau E_n/\hbar}$. If one now lets the imaginary time $\tau$ approach to infinity, then only the information on the ground state will be kept. More precisely, we have for the density

$$\phi_0^2(q) = \lim_{\tau\to\infty} e^{-\tau E_0/\hbar}K(q,\tau;q,0), \tag{4.7}$$

where $q_0 = q$ (the periodic boundary condition) is also used. Since the ground state wave function should be normalized, we obtain $\phi_0^2(q) = K(q,\tau;q,0)/\int_{-\infty}^{\infty}\mathrm{d}qK(q,\tau;q,0)$. It is very important to remember that in order to evaluate the wave function, the periodic condition and the imaginary-time scheme are adopted. In the followed steps, one can do the standard Monte Carlo simulation like the Metropolis to fulfill the above algorithm by treating the fact appeared in the exponential

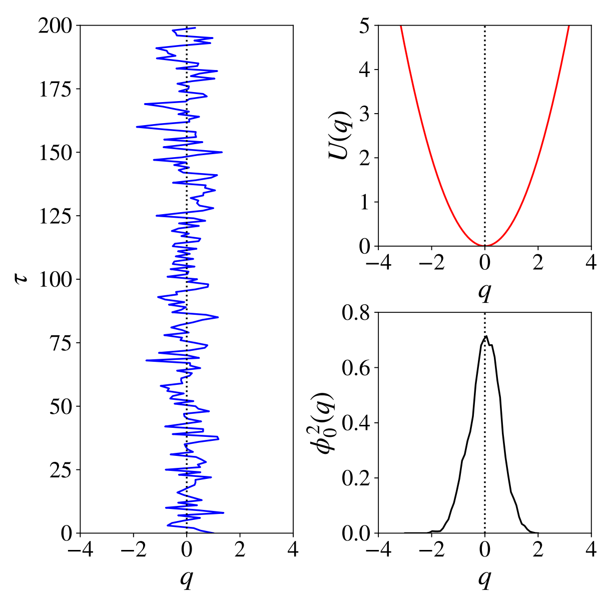



Fig. D: Monte Carlo simulation for path integral for harmonic oscillator (adopting Metropolis algorithm).

the effective energy. In Fig. D, we show the calculated results using the Metropolis algorithm for the harmonic oscillator with $U(q) = q^2/2$, here the left panel is the path in the imaginary time, and the right-lower panel shows the squared wave function $\phi_0^2(q)$. One can also study the ground state wave function of a double-well function, e.g., $U(q) = q^4 + \lambda q^2$ where $\lambda < 0$ is an control parameter. The non-trivial vacuum states of this function are given by $q = \pm(-\lambda/2)^{1/2}$. In Fig. E the paths in the imaginary-time domain with decreasing $\lambda$ (from left to right) are shown. As one can see when the control parameter becomes more negative, the two equilibrium configurations $\sqrt{\lambda/2}$ and $-\sqrt{\lambda/2}$ become more separable. Fig. F shows the squared wave functions with three typical $\lambda$'s, i.e., $\lambda = 0, -6$ and $-12$ (from left to right). The squared wave function in the left panel is very similar as the one obtained for the harmonic oscillator since the overall shape of $q^4$ is similar like that of $q^2$. However as a nonnegative $\lambda$ emerges, the double-peak wave function also emerges naturally. The imaginary-time formalism is the foundation of many quantum Monte Carlo algorithms.

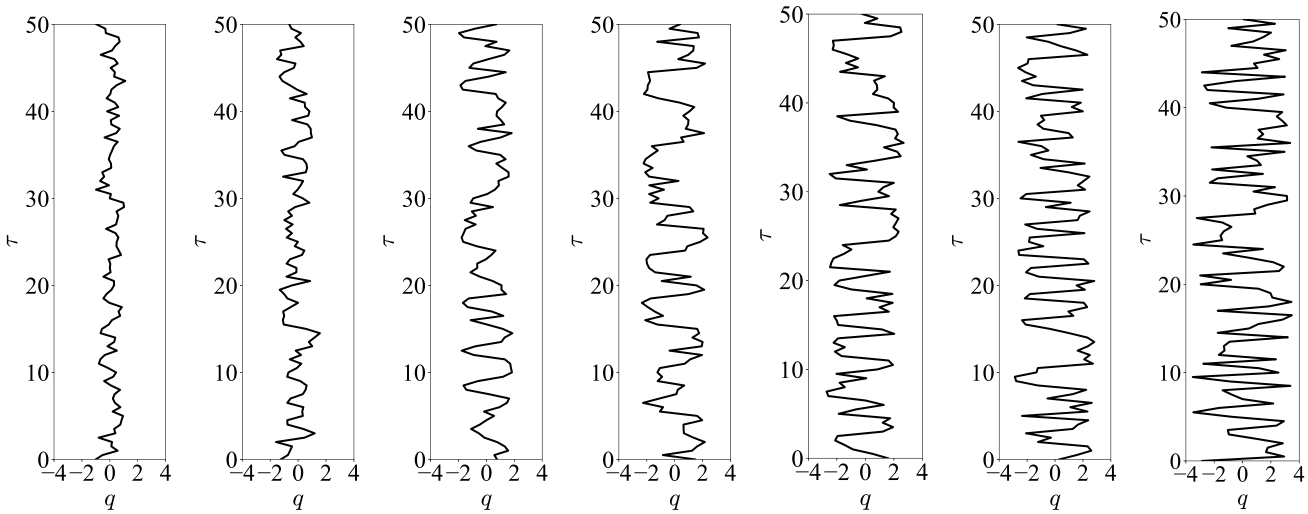



Fig. E: Paths in the imaginary-time domain with decreasing $\lambda$ (from left to right) of the potential $U(q) = q^4 + \lambda q^2$ (with $\lambda < 0$).

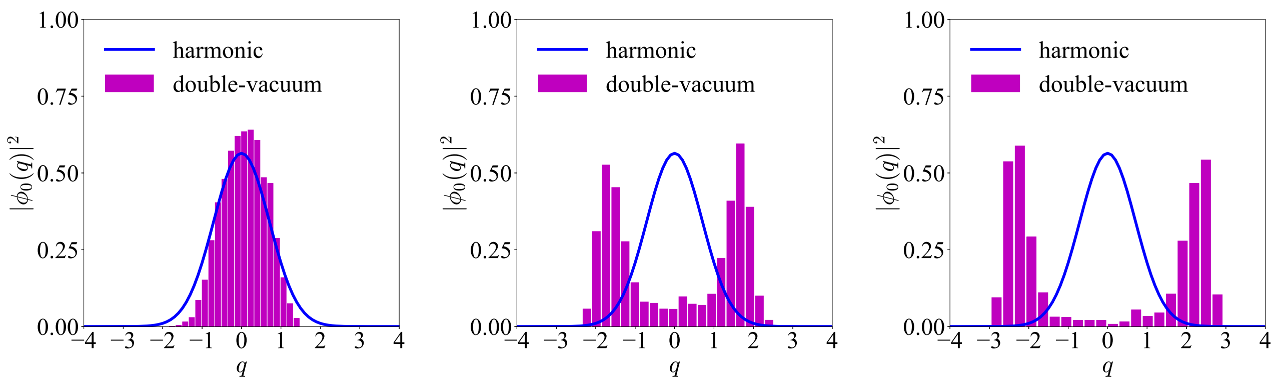



Fig. F: Squared wave functions with $\lambda = 0, -6$ and $-12$.

**EXERCISE 18**: How to obtain the ground state energy $E_0$ from evaluating the imaginary-time path integral?
**EXERCISE 19**: For the harmonic oscillator, the first-excited energy level could be obtained from,

$$E_1 - E_0 = \Delta E = -\frac{1}{\epsilon} \ln\left(\frac{\langle q(0)q(\tau+\epsilon)\rangle}{\langle q(0)q(\tau)\rangle}\right). \tag{4.8}$$

Explain this formula. Then evaluate the first-excited energy in the harmonic oscillator for $U(q) = q^2/2$.

## E *Matsubara Frequency, Thermal Mass of a Scalar Field

RELEVANT REFERENCES:

- J. Kapusta, *Quantum Field Theory at Finite Temperature*, Cambridge University Press, 1989, Chapters 2 and 3.
- M. Laine and A. Vuorinen, *Basics of Thermal Field Theory: A Tutorial on Perturbative Computations*, Springer International Publishing, 2016, Chapters 2 and 3.

The imaginary-time formalism of the last section (e.g., Eq. (4.5)) could be generalized to the situation of a continuous field theory. For example, for a real scalar field with Lagrangian (we adopt $\hbar = c = 1$),

$$\mathcal{L}_0 = \frac{1}{2}\partial_\mu\phi\partial^\mu\phi - \frac{1}{2}m^2\phi^2 = \frac{1}{2}\left[(\partial_t\phi)^2 - (\nabla\phi)^2 - m^2\phi\right], \tag{5.1}$$

one can obtain the partition function,

$$\boxed{Z_0 = \mathrm{tr}\left[e^{-\beta(H_0-\mu N)}\right] = \int \mathrm{d}\phi\langle\phi|e^{-\beta(H_0-\mu N)}|\phi\rangle = \int \mathcal{D}\pi\int_{\phi(\mathbf{x},0)=\phi(\mathbf{x},\beta)}\mathcal{D}\phi\exp\left(-\int_0^\beta \mathrm{d}\tau\int \mathrm{d}\mathbf{x}(\mathcal{H}_0 - \mu\mathcal{N} - i\pi\partial_\tau\phi)\right),} \tag{5.2}$$

where $\tau = it$, $\pi = \partial_t\phi$ is the canonical momentum and $\mathcal{H}_0 = \pi\partial_t\phi - \mathcal{L}_0 = [\pi^2 + (\nabla\phi)^2 + m^2\phi^2]/2$. Notice the periodic boundary condition $\phi(\mathbf{x},0) = \phi(\mathbf{x},\beta)$. After integrating the momentum part, we shall obtain

$$\boxed{Z_0 = \overline{\mathcal{N}}\int\mathcal{D}\phi\exp\left(-\int_0^\beta\mathrm{d}\tau\int\mathrm{d}\mathbf{x}\mathcal{L}_0\right) = \overline{\mathcal{N}}\int\mathcal{D}\phi e^{-S_0} \sim \int\mathcal{D}\phi e^{-S_0},} \tag{5.3}$$

here $\overline{\mathcal{N}}$ is an integration constant (due to the momentum). The Lagrangian appearing in Eq. (5.3) is Euclidean, i.e.,

$$\mathcal{L}_{0,\mathrm{E}} = \frac{1}{2}\left[(\partial_\tau\phi)^2 + (\nabla\phi)^2 + m^2\phi^2\right]. \tag{5.4}$$

However, we will frequently omit the subscript "E".

We introduce $X \equiv (x^0,\mathbf{x}) = (t,\mathbf{x}) = (-i\tau,\mathbf{x})$ and $K \equiv (k^0,\mathbf{k}) = (-i\omega_n,\mathbf{k})$, here $\omega_n$ is called the Matsubara frequency. The Fourier transform of $\phi(X)$ is defined as

$$\phi(X) = \frac{1}{\sqrt{TV}}\sum_K e^{-iK\cdot X}\phi(K) = \frac{1}{\sqrt{TV}}\sum_{n,\mathbf{k}} e^{i(\omega_n\tau+\mathbf{k}\cdot\mathbf{x})}\phi(K), \tag{5.5}$$

where $K\cdot X = KX = k^0x^0 - \mathbf{k}\cdot\mathbf{x}$, we also have $\phi(-K) = \phi^*(K)$ since $\phi(X)$ is real. The boundary condition $\phi(0,\mathbf{x}) = \phi(\beta,\mathbf{x})$ gives $e^{i\omega_n\beta} = 1$, or

$$\boxed{\omega_n = 2\pi nT, \quad n\in\mathrm{Z}.} \tag{5.6}$$

Now, the action in momentum space becomes,

$$\boxed{S_0 = \int_X\mathcal{L}_0 = \frac{1}{2}\int_X\left[(\partial_\tau\phi)^2 + (\nabla\phi)^2 + m^2\phi^2\right] = \frac{1}{2}\sum_K\phi(-K)\frac{D_0^{-1}(K)}{T^2}\phi(K), \quad \int_X \equiv \int_0^\beta\mathrm{d}\tau\int\mathrm{d}\mathbf{x},} \tag{5.7}$$

where $D_0(K)$ is the free propagator in momentum space,

$$\boxed{D_0^{-1}(K) = \omega_n^2 + |\mathbf{k}|^2 + m^2,} \tag{5.8}$$

since

$$\begin{aligned}\int_X(\partial_\tau\phi)^2 &= \frac{1}{TV}\int_X\sum_{K,Q}\left[\partial_\tau e^{i(\omega_n\tau+\mathbf{k}\cdot\mathbf{x})}\phi(K)\right]\left[\partial_\tau e^{i(\omega_m\tau+\mathbf{q}\cdot\mathbf{x})}\phi(Q)\right]\\ &= -\frac{1}{TV}\int_X\sum_{K,Q}\omega_n\omega_m e^{-i(K+Q)X}\phi(K)\phi(Q) = \frac{1}{T^2}\sum_K\omega_n^2\phi(-K)\phi(K),\end{aligned} \tag{5.9}$$

$$\begin{aligned}\int_X(\nabla\phi)^2 &= \frac{1}{TV}\int_X\sum_{K,Q}\left[\nabla e^{i(\omega_n\tau+\mathbf{k}\cdot\mathbf{x})}\phi(K)\right]\left[\nabla e^{i(\omega_m\tau+\mathbf{q}\cdot\mathbf{x})}\phi(Q)\right]\\ &= -\frac{1}{TV}\int_X\sum_{K,Q}\mathbf{k}\cdot\mathbf{q}e^{-i(K+Q)X}\phi(K)\phi(Q) = \frac{1}{T^2}\sum_K|\mathbf{k}|^2\phi(-K)\phi(K),\end{aligned} \tag{5.10}$$

$$\begin{aligned}\int_X m^2\phi^2 &= \frac{m^2}{TV}\int_X\sum_{K,Q}\left[e^{i(\omega_n\tau+\mathbf{k}\cdot\mathbf{x})}\phi(K)\right]\left[e^{i(\omega_m\tau+\mathbf{q}\cdot\mathbf{x})}\phi(Q)\right]\\ &= -\frac{m^2}{TV}\int_X\sum_{K,Q}e^{-i(K+Q)X}\phi(K)\phi(Q) = \frac{m^2}{T^2}\sum_K\phi(-K)\phi(K).\end{aligned} \tag{5.11}$$

The partition function is given by

$$\boxed{Z_0 = \overline{\mathcal{N}} \int \mathcal{D}\phi(K) \exp\left[-\frac{1}{2}\sum_K \phi^*(K) \frac{D_0^{-1}(K)}{T^2} \phi(K)\right].} \tag{5.12}$$

Considering the multi-dimensional Gaussian integration $\int \mathrm{d}q_1 \cdots \mathrm{d}q_d e^{-qXq/2} = \sqrt{(2\pi)^d / \det X}$, we further write

$$\boxed{Z_0 = \left(\det \frac{D_0^{-1}(K)}{T^2}\right)^{-1/2},} \tag{5.13}$$

where another constant is omitted for simplicity. Consequently,

$$\boxed{\ln Z_0 = -\frac{1}{2} \ln \det \frac{D_0^{-1}(K)}{T^2} = -\frac{1}{2} \ln \prod_K \frac{D_0^{-1}(K)}{T^2} = -\frac{1}{2} \sum_K \ln \frac{D_0^{-1}(K)}{T^2}.} \tag{5.14}$$

By using the theorem of residue one can perform the sum over Matsubara frequency, then

$$\boxed{\ln Z_0 = -\frac{1}{2} \sum_{n,\mathbf{k}} \frac{\omega_n^2 + \epsilon_k^2}{T^2} = -V \int \frac{\mathrm{d}\mathbf{k}}{(2\pi)^3} \left[\frac{\epsilon_k}{2T} + \ln\left(1 - e^{-\epsilon_k/T}\right)\right], \ \epsilon_k = \sqrt{k^2 + m^2},} \tag{5.15}$$

the first term here is divergent (zero-point energy).

**EXERCISE 20**: Argue that $\phi(K)$ is dimensionless, and show that $\int_X e^{iKX} = (V/T)\delta_{K0}$.
**EXERCISE 21**: Finish the process leading to Eq. (5.15) using complex integration techniques.
**EXERCISE 22**: Thermodynamic quantities can be obtained via the partition function,

$$\Omega_0 = -T \ln Z_0 = TV \int \frac{\mathrm{d}\mathbf{k}}{(2\pi)^3} \left[\frac{\epsilon_k}{2T} + \ln\left(1 - e^{-\epsilon_k/T}\right)\right], \ P_0 = T\frac{\partial \ln Z_0}{\partial V} = -T \int \frac{\mathrm{d}\mathbf{k}}{(2\pi)^3} \left[\frac{\epsilon_k}{2T} + \ln\left(1 - e^{-\epsilon_k/T}\right)\right], \tag{5.16}$$

$$E_0 = -\frac{\partial \ln Z_0}{\partial \beta} = V \int \frac{\mathrm{d}\mathbf{k}}{(2\pi)^3} \left[\frac{\epsilon_k}{2} + \frac{\epsilon_k}{1 - e^{-\epsilon_k/T}}\right], \ C_V = \left(\frac{\partial E_0}{\partial T}\right)_V = V \int \frac{\mathrm{d}\mathbf{k}}{(2\pi)^3} \frac{\epsilon_k^2 e^{-\epsilon_k/T}}{T^2(1 - e^{-\epsilon_k/T})^2}. \tag{5.17}$$

Discuss their high- and low-temperature behaviors. Show that after omitting the vacuum part, the pressure at high temperature is

$$P_0 \approx \frac{\pi^2 T^4}{90} - \frac{m^2 T^2}{24} + \frac{m^3 T}{12\pi} + \frac{m^4}{2(4\pi)^2}\left(\ln \frac{m e^\gamma}{4\pi T} - \frac{3}{4}\right) - \frac{m^6 \zeta(3)}{3(4\pi)^4 T^2} + \cdots, \tag{5.18}$$

here $\gamma$ is the Euler constant. What is its low-temperature limit?

The propagator in coordinate space can be obtained as,

$$\begin{aligned} D_0(X) = \langle\phi(X)\phi(0)\rangle_0 &= \left\langle \frac{1}{TV} \sum_{K,Q} e^{-iKX} \phi(K)\phi(Q) \right\rangle_0 = \frac{T}{V}\frac{1}{T^2} \left\langle \sum_{K,Q} e^{-iKX} \phi(K)\phi(Q) \right\rangle_0 \\ &= \frac{T}{V} \sum_K e^{-iKX} \frac{1}{T^2} \sum_Q \langle\phi(K)\phi(Q)\rangle_0 = \frac{T}{V} \sum_K e^{-iKX} \frac{1}{T^2} \langle\phi(K)\phi(-K)\rangle_0, \end{aligned} \tag{5.19}$$

where in the last step one considers the fact that the ensemble average is nonzero only when $K + Q = 0$:

$$\langle\phi(P)\phi(Q)\rangle_0 = \frac{\prod_K \int \mathrm{d}\phi(K) \exp\left[-\frac{1}{2}\phi(-K)\frac{D_0^{-1}(K)}{T^2}\phi(K)\right]\phi(P)\phi(Q)}{\prod_K \int \mathrm{d}\phi(K) \exp\left[-\frac{1}{2}\phi(-K)\frac{D_0^{-1}(K)}{T^2}\phi(K)\right]} = \delta_{P+Q,0}. \tag{5.20}$$

Since

$$D_0(Q) = \frac{1}{T^2} \frac{\prod_K \int \mathrm{d}\phi(K) \exp\left[-\frac{1}{2}\phi(-K)\frac{D_0^{-1}(K)}{T^2}\phi(K)\right]\phi(Q)\phi(-Q)}{\prod_K \int \mathrm{d}\phi(K) \exp\left[-\frac{1}{2}\phi(-K)\frac{D_0^{-1}(K)}{T^2}\phi(K)\right]} = \frac{1}{T^2}\langle\phi(Q)\phi(-Q)\rangle_0, \tag{5.21}$$

we have

$$D_0(X) = \frac{T}{V}\sum_K e^{-iKX} D_0(Q), \tag{5.22}$$

which could be further written as using Eq. (5.8),

$$\boxed{D_0(X) = T\sum_n \int \frac{\mathrm{d}\mathbf{k}}{(2\pi)^3}\frac{e^{i\omega_n\tau + i\mathbf{k}\cdot\mathbf{x}}}{\omega_n^2+\epsilon_k^2}, \quad \omega_n = 2\pi nT.} \tag{5.23}$$

**EXERCISE 23**: Prove that in $d$ dimensions, $D_0(X)$ is given by

$$D_0(X) = \int \frac{\mathrm{d}^d\mathbf{k}}{(2\pi)^d}\frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{2\epsilon_k}\frac{\cosh[(\beta/2-|x^0|)\epsilon_k]}{\sinh(\beta\epsilon_k/2)}\bigg|_{\epsilon_k=\sqrt{|\mathbf{k}|^2+m^2}}. \tag{5.24}$$

Discuss its short- and large-distance behaviors.

Interaction may introduce extra novel features to the problem. Here, we consider the $\phi^4$ interaction in the form of $\mathcal{L} = \mathcal{L}_0 + \mathcal{L}_{\text{int}} = 2^{-1}\partial_\mu\phi\partial^\mu\phi - 2^{-1}m^2\phi^2 - \lambda\phi^4$. The partition function is similarly given as (the in-front constant is omitted),

$$Z = \int \mathcal{D}\phi e^{-S}, \quad S = S_0 + S_{\text{int}} = \int_X \mathcal{L}_0 + \int_X \mathcal{L}_{\text{int}}, \quad S_{\text{int}} = \lambda\int_X \phi^4. \tag{5.25}$$

Assuming $\lambda$ is small, then

$$\boxed{\ln Z = \ln\int\mathcal{D}\phi e^{-S_0-S_{\text{int}}} = \ln\left(\int\mathcal{D}\phi e^{-S_0}\sum_{n=0}^{\infty}\frac{(-S_{\text{int}})^n}{n!}\right),} \tag{5.26}$$

which becomes after subtracting and adding $\ln Z_0$,

$$\boxed{\ln Z = \ln Z_0 + \ln\left(\frac{\int\mathcal{D}\phi e^{-S_0}\sum_{n=0}^{\infty}\frac{(-S_{\text{int}})^n}{n!}}{\int\mathcal{D}\phi e^{-S_0}}\right) = \ln Z_0 + \ln Z_{\text{int}},} \tag{5.27}$$

where

$$\boxed{\ln Z_{\text{int}} \equiv \ln\left(1+\sum_{n=1}^{\infty}\frac{1}{n!}\frac{1}{\int\mathcal{D}\phi e^{-S_0}(-S_{\text{int}})^n}\int\mathcal{D}\phi e^{-S_0}\right) = \ln\left(1+\sum_{n=1}^{\infty}\frac{\langle(-S_{\text{int}})^n\rangle_0}{n!}\right).} \tag{5.28}$$

Here, $\langle\cdots\rangle_0$ implies that the ensemble average is taken in the free Lagrangian. For example, we have to order $\lambda^3$ that

$$\begin{aligned}\ln Z_{\text{int}} &\approx \ln\left(1-\langle S_{\text{int}}\rangle_0 + \frac{\langle S_{\text{int}}^2\rangle_0}{2} - \frac{\langle S_{\text{int}}^3\rangle_0}{6}\right)\\ &\approx -\langle S_{\text{int}}\rangle_0 + \frac{1}{2}\left(\langle S_{\text{int}}^2\rangle_0 - \langle S_{\text{int}}\rangle_0^2\right) - \frac{1}{6}\left(\langle S_{\text{int}}^3\rangle_0 - 3\langle S_{\text{int}}\rangle_0\langle S_{\text{int}}^2\rangle_0 + 2\langle S_{\text{int}}\rangle_0^3\right).\end{aligned} \tag{5.29}$$

Let's discuss in more details the perturbation at linear order of $\lambda$. Since,

$$\langle S_{\text{int}}\rangle_0 = \lambda\frac{\int\mathcal{D}\phi e^{-S_0}\int_X\phi^4(X)}{\int\mathcal{D}\phi e^{-S_0}}, \tag{5.30}$$

where

$$e^{-S_0} = \exp\left(-\frac{1}{2}\sum_K\phi(-K)\frac{D_0^{-1}(K)}{T^2}\phi(K)\right) = \prod_K\exp\left(-\frac{1}{2}\phi(-K)\frac{D_0^{-1}(K)}{T^2}\phi(K)\right), \tag{5.31}$$

$$\int_X\phi^4(X) = \frac{1}{T^2V^2}\sum_{K_1,\cdots,K_4}\int_X e^{i(K_1+\cdots+K_4)X}\phi(K_1)\cdots\phi(K_4) = \frac{1}{T^3V}\sum_{K_1,\cdots,K_4}\delta(K_1+\cdots+K_4)\phi(K_1)\cdots\phi(K_4), \tag{5.32}$$

we have

$$\boxed{\langle S_{\rm int}\rangle_0 = \frac{\lambda}{T^3V}\frac{\sum\limits_{K_1,\cdots,K_4}\delta(K_1+\cdots+K_4)\prod\limits_K\int \mathrm{d}\phi(K)\exp\left(-\frac{1}{2}\phi(-K)\frac{D_0^{-1}(K)}{T^2}\phi(K)\right)\phi(K_1)\cdots\phi(K_4)}{\prod\limits_K\int \mathrm{d}\phi(K)\exp\left(-\frac{1}{2}\phi(-K)\frac{D_0^{-1}(K)}{T^2}\phi(K)\right)}.} \tag{5.33}$$

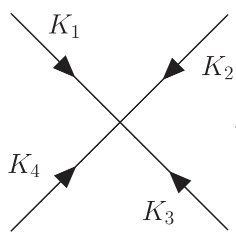
In order to simplify this expression, we notice the integration is nonzero only when $K_1$,$K_2$,$K_3$ and $K_4$ cancel each other. There are three choices on contracting two momenta (lines) from four, therefore

$$\boxed{\begin{aligned}\langle S_{\rm int}\rangle_0 =& \frac{3\lambda}{T^3V}\sum_{Q,P}\frac{\prod\limits_K\int \mathrm{d}\phi(K)\exp\left(-\frac{1}{2}\phi(-K)\frac{D_0^{-1}(K)}{T^2}\phi(K)\right)\phi(-Q)\phi(Q)\phi(-P)\phi(P)}{\prod\limits_K\int \mathrm{d}\phi(K)\exp\left(-\frac{1}{2}\phi(-K)\frac{D_0^{-1}(K)}{T^2}\phi(K)\right)}\\ =& \frac{3\lambda}{T^3V}\left[\sum_Q\frac{\prod\limits_Q\int \mathrm{d}\phi(Q)\exp\left(-\frac{1}{2}\phi(-Q)\frac{D_0^{-1}(Q)}{T^2}\phi(Q)\right)\phi(Q)\phi(-Q)}{\prod\limits_Q\int \mathrm{d}\phi(Q)\exp\left(-\frac{1}{2}\phi(-Q)\frac{D_0^{-1}(Q)}{T^2}\phi(Q)\right)}\right]^2.\end{aligned}} \tag{5.34}$$

Using the expression for $D_0(Q)$ leads us to

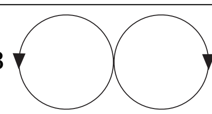
$$\boxed{\ln Z_{\rm int}^{(1)} = -\langle S_{\rm int}\rangle_0 = -3\lambda\frac{T}{V}\left[\sum_Q D_0(Q)\right]^2.} \tag{5.35}$$

Graphically, we use the following diagram to represent the interaction $\lambda\phi^4$ (vertex),




. (5.36)

Contracting the four external lines then gives the corresponding contribution,

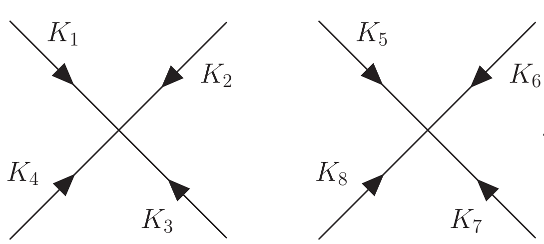
$$-\langle S_{\rm int}\rangle_0 = -3\lambda\frac{T}{V}\left[\sum_Q D_0(Q)\right]^2 = 3$$  . (5.37)

Here, each vertex induces the coupling constant $-\lambda$ one time and each closed loop corresponds to $T/V\sum_Q D_0(Q)$. Moreover, momentum conservation gives the factor $V/T\delta(K_{\rm in}-K_{\rm out})$, and “3” is the combinatorial factor.

There is only one linked diagram in the first-order approximation. The un-linked diagrams in $\ln Z$ would be canceled with each other, e.g., in the second-order approximation, we have

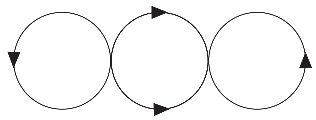
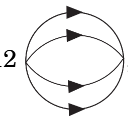
$$\ln Z_{\rm int}^{(2)} = \frac{1}{2}\left(\langle S_{\rm int}^2\rangle_0 - \langle S_{\rm int}\rangle_0^2\right). \tag{5.38}$$

Here the diagram corresponding to $\langle S_{\rm int}^2\rangle_0$ should be constructed from $(-\lambda\phi)^2$, namely from the following diagrams,

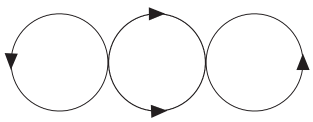



. (5.39)

One possibility is contracting the left and diagram separably and obtaining two bubble diagrams, which cancel the contribution from the term $\langle S_{\text{int}}\rangle_0^2$, and the remaining contribution is given by

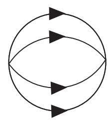
$$\ln Z^{(2)}_{\text{int}} = 36$$

$$+\,12$$

$$, \tag{5.40}$$

here "36" and "12" are other related combinatorial factors. In particular, we have the following "translations",



$$=(-\lambda)^2\left(\frac{T}{V}\right)^4\left(\frac{V}{T}\right)^2\sum_{K_1,\cdots,K_4}\delta(K_2+K_3)D_0(K_1)\cdots D_0(K_4)$$

$$=\lambda^2\frac{T^2}{V^2}\left[\sum_K D_0(K)\right]^2\sum_{K_2,K_3}\delta(K_2+K_3)D_0(K_2)D_0(K_3), \tag{5.41}$$

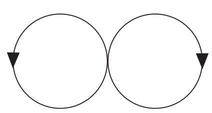
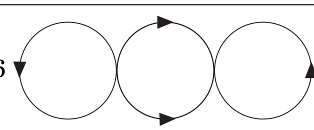
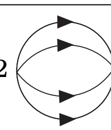


$$=(-\lambda)^2\left(\frac{T}{V}\right)^4\left(\frac{V}{T}\right)^2\sum_{K_1,\cdots,K_4}\delta(K_1+\cdots+K_4)D_0(K_1)\cdots D_0(K_4). \tag{5.42}$$

One can prove mathematically that

$$\boxed{\ln Z_{\text{int}} = \sum_{n=1}^{\infty}\frac{(-)^n\langle S^n_{\text{int}}\rangle_{0,\text{connected}}}{n!},} \tag{5.43}$$

which is called the linked-cluster theorem. Consequently, we have to order $\lambda^2$ that,

$$\ln Z_{\text{int}} \approx 3$$

$$+\,36$$

$$+\,12$$

$$+\,\mathcal{O}(\lambda^3). \tag{5.44}$$

We will see in the following that these diagrams are not complete, and there would be terms proportional to $\lambda^{3/2}$.

The full propagator could be decomposed into the free part and the interaction part (i.e., self-energy),

$$\boxed{D^{-1}(K) = D_0^{-1}(K)+\Pi(K).} \tag{5.45}$$

The connection between $\Pi$ and $\ln Z_{\text{int}}$ could be established as follows. Since $\ln Z = \ln\int\mathcal{D}\phi e^{-S_0-S_{\text{int}}}$, we have

$$\begin{aligned}\frac{\delta\ln Z}{\delta D_0^{-1}(Q)} &= \frac{1}{\int\mathcal{D}\phi e^{-S_0-S_{\text{int}}}}\frac{\delta}{\delta D_0^{-1}(Q)}\int\mathcal{D}\phi e^{-S_0}e^{-S_{\text{int}}}\\ &= \frac{1}{\int\mathcal{D}\phi e^{-S_0-S_{\text{int}}}}\frac{\delta}{\delta D_0^{-1}(Q)}\prod_K\int \mathrm{d}\phi(K)\exp\left(-\frac{1}{2}\phi(-K)\frac{D_0^{-1}(K)}{T^2}\phi(K)\right)e^{-S_{\text{int}}}\\ &= -\frac{1}{2T^2}\frac{\int\mathcal{D}\phi e^{-S_0-S_{\text{int}}}\phi(-Q)\phi(Q)}{\int\mathcal{D}\phi e^{-S_0-S_{\text{int}}}} = -\frac{1}{2}D(Q),\end{aligned} \tag{5.46}$$

therefore

$$\boxed{D(Q) = -2\frac{\delta\ln Z}{\delta D_0^{-1}} = 2D_0^2\frac{\delta\ln Z}{\delta D_0}.} \tag{5.47}$$

According to the definition of (5.45), we obtain $D=[D_0^{-1}+\Pi]^{-1}=D_0[1+D_0\Pi]^{-1}$. From the relation (5.47) we then have

$$\boxed{\frac{1}{1+\Pi D_0} = 2D_0\frac{\delta\ln Z}{\delta D_0}.} \tag{5.48}$$

By expanding both sides of Eq. (5.48) over $\lambda$ and writing the self-energy in the series of $\Pi = \sum_{n=1}^{\infty} \Pi_n$, one can find that $\Pi_n$ is proportional to $\lambda^n$. For instance, we have at order $\lambda^2$ that,

$$\frac{1}{1+\Pi D_0} = 1 - D_0\Pi_1 - D_0\Pi_2 + D_0\Pi_1 D_0\Pi_1 + \mathcal{O}(\lambda^3). \tag{5.49}$$

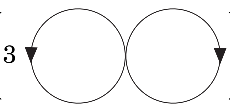
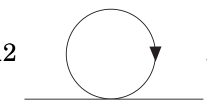
Eq. (5.14) gives $\delta \ln Z_0/\delta D_0 = 2^{-1} D_0^{-1}$, and therefore

$$2D_0 \frac{\delta \ln Z}{\delta D_0} = 2D_0 \left( \frac{\delta \ln Z_0}{\delta D_0} + \frac{\delta \ln Z_{\text{int}}}{\delta D_0} \right) = 1 + 2D_0 \frac{\delta \ln Z_{\text{int}}}{\delta D_0} \approx 1 + 2D_0 \left[ -\frac{\delta \langle S_{\text{int}} \rangle_0}{\delta D_0} + \frac{1}{2} \frac{\delta(\langle S_{\text{int}}^2 \rangle_0 - \langle S_{\text{int}} \rangle_0^2)}{\delta D_0} \right]. \tag{5.50}$$

We consequently obtain,

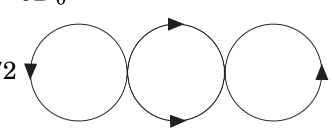
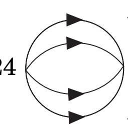
$$\boxed{\Pi_1 + \Pi_2 - \Pi_1 D_0 \Pi_1 + \cdots = -2\frac{\delta \ln Z_{\text{int}}}{\delta D_0}, \ \text{ with } \ \Pi_1 = 2\frac{\delta \langle S_{\text{int}} \rangle_0}{\delta D_0}, \ \ \Pi_2 - \Pi_1 D_0 \Pi_1 = -\frac{\delta(\langle S_{\text{int}}^2 \rangle_0 - \langle S_{\text{int}} \rangle_0^2)}{\delta D_0}.} \tag{5.51}$$

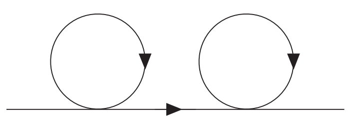
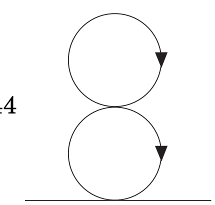
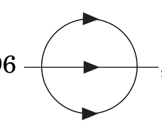
One can express the self-energy $\Pi_1$ graphically as

$$\Pi_1 = 6\lambda \frac{T}{V} \frac{\delta}{\delta D_0} \left[ \sum_K D_0(K) \right]^2 = 12\lambda \frac{T}{V} \sum_K D_0(K) = -2 \frac{\delta}{\delta D_0} \left( 3 \right.$$

$$\left. \right) = -12$$

$$. \tag{5.52}$$

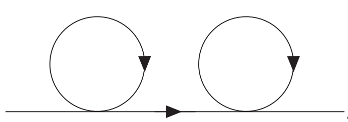
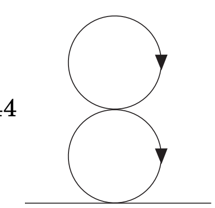
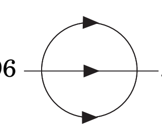
We find calculating the functional derivative with respect to the propagator is equivalent to cutting a line. Similarly,

$$\Pi_2 - \Pi_1 D_0 \Pi_1 = -\frac{\delta(\langle S_{\text{int}}^2 \rangle_0 - \langle S_{\text{int}} \rangle_0^2)}{\delta D_0} \tag{5.53}$$

$$= -\frac{\delta}{\delta D_0} \left( 72 \right.$$

$$+ 24$$

$$\left. \right) \tag{5.54}$$

$$= -144$$

$$-144$$

$$-96$$

$$, \tag{5.55}$$

therefore

$$\Pi_1 D_0 \Pi_1 = 144$$

$$, \quad \Pi_2 = -144$$

$$-96$$

$$. \tag{5.56}$$

The self-energy is in fact constructed from the one–particle–irreducible (1PI), i.e.,

$$\boxed{\Pi = -2 \left( \frac{\delta \ln Z_{\text{int}}}{\delta D_0} \right)_{\text{1PI}}.} \tag{5.57}$$

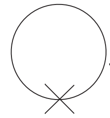
Check $\Pi_1$ and $\Pi_2$ for this relation.

We calculate the contribution from $\Pi_1$ to the pressure. In order to do that, we first write out the expression for $\Pi_1$,

$$\Pi_1 = 12\lambda \frac{T}{V} \sum_K \frac{1}{\omega_n^2 + \epsilon_k^2} = \Pi_1^{\text{vac}} + \Pi_1^T = 6\lambda \int \frac{\mathbf{dk}}{(2\pi)^3} \frac{1}{\epsilon_k} + 12\lambda \int \frac{\mathbf{dk}}{(2\pi)^3} \frac{f(\epsilon_k)}{\epsilon_k}, \quad f(\epsilon_k) = \frac{1}{e^{\epsilon_k/T} - 1}. \tag{5.58}$$

The temperature-dependent part is convergent while the vacuum contribution diverges. We can remove the divergent vacuum contribution by using the renormalized self-energy, $\Pi_1^{\text{ren}} = \Pi_1 - \Pi_1^{\text{vac}}$. Then the modified propagator is given by $D^{-1}(K) = \omega_n^2 + k^2 + m^2 + \Pi_1$. We see that the self-energy plays a similar role as the mass squared term in the Lagrangian, and we can account for this effect by adding the a contribution in the original Lagrangian as $\mathcal{L} \to \mathcal{L} - 2^{-1}\delta m^2 \phi^2$. This added new term could be treated as another interaction and $\delta m^2$ has the same order as $\lambda$. Its graph is represented as

$$\delta m^2 \langle \phi^2 \rangle_0 = \quad . \tag{5.59}$$



The cutting rule then gives the corresponding contribution to the self-energy as

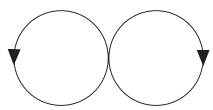
$$\delta m^2 = \quad . \tag{5.60}$$

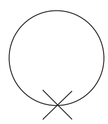
In this sense, we can obtain finite result by selecting the renormalized scheme $\delta m^2 = -\Pi_1^{\text{vac}}$.

For massless Boson ($m = 0$), which is equivalent to high temperature $T \gg m$, we have

$$\boxed{\Pi_1^{\text{ren}} = 12\lambda \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{f(\epsilon_k)}{\epsilon_k} \approx \lambda T^2,} \tag{5.61}$$

where the relation $\int_0^\infty x dx/(e^x - 1) = \pi^2/6$ is used. We see that the massless Boson acquires a thermal mass $\lambda T^2$ at high temperatures. The $\ln Z_{\text{int}}$ at order $\lambda$ is given by including the mass-correction term as,





$$\begin{aligned}\ln Z_{\text{int}}^{(1)} = 3 \quad - \frac{1}{2} \quad &= -3\lambda \frac{V}{T}\left[\frac{T}{V}\sum_Q D_0(Q)\right]^2 - \frac{1}{2}\delta m^2 \sum_Q D_0(Q) \\ &= -\frac{V}{T}\frac{1}{48\lambda}\left(\Pi_1^{\text{vac}} + \Pi_1^T\right)^2 + \frac{V}{T}\frac{1}{24\lambda}\Pi_1^{\text{vac}}\left(\Pi_1^{\text{vac}} + \Pi_1^T\right) = \frac{V}{T}\frac{1}{48\lambda}\left(\Pi_1^{\text{vac},2} - \Pi_1^{T,2}\right),\end{aligned} \tag{5.62}$$

therefore we obtain (after removing the vacuum part),

$$\boxed{\frac{T}{V}\ln Z_{\text{int}}^{(1)} = -3\lambda\left[\int \frac{d\mathbf{k}}{(2\pi)^3}\frac{f(\epsilon_k)}{\epsilon_k}\right]^2 \approx -\frac{\lambda T^4}{48}.} \tag{5.63}$$

The corresponding expression for the pressure is then,

$$\boxed{P = \frac{\pi^2 T^4}{90}\left(1 - \frac{15}{8}\frac{\lambda}{\pi^2} + \cdots\right).} \tag{5.64}$$

We have already seen that the first-order perturbation adds a thermal mass $\lambda T^2$ to the massless particle. At low momentum/energy (near the thermal mass scale), i.e., $\omega_n^2, |\mathbf{k}|^2 \sim \lambda T^2$, the free propagator $D_0^{-1} = \omega_n^2 + k^2$ itself is on the order of $\lambda T^2$. However, the contribution from the self-energy is also on such order, implying the above perturbative calculation is unreasonable. Actually, we need to consider an infinite series of graphs to remove the infrared divergence, a technique sometimes called resummation. The full propagator should be used instead of the free one, i.e.,

$$\Pi = 12\lambda \frac{T}{V}\sum_K D(K) = 12\lambda \frac{T}{V}\sum_K \frac{1}{D_0^{-1}(K) + \Pi}, \tag{5.65}$$

this is a self-consistent equation for $\Pi$. We expand the term above to obtain,

$$\frac{1}{D_0^{-1}(K) + \Pi} = D_0 \sum_{n=0}^{\infty}(-\Pi D_0)^n, \quad \Pi = 12\lambda \frac{T D_0}{V}\sum_K \sum_{n=0}^{\infty}(-\Pi D_0)^n. \tag{5.66}$$

If one uses $\Pi_1$ to approximate $\Pi$ in (5.65) then there would be a large loop on which $n$ small loops are attached. Such diagram is often called a daisy diagram. Iterating the process further, one should obtain the so-called super-daisy diagram. We would like to point out that although there are many many loops in the diagram the overall structure of the self-energy is still one-loop. We now write Eq. (5.65) in the following more apparent form,

$$\Pi = 12\lambda \int \frac{d\mathbf{k}}{(2\pi)^3} T \sum_n \frac{1}{\omega_n^2 + k^2 + \Pi} = 12\lambda \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{f\left(\sqrt{k^2 + \Pi}\right)}{\sqrt{k^2 + \Pi}}, \tag{5.67}$$

where the sum over Matsubara is used and the zero-temperature is removed. By introducing a new integration variable $x = \sqrt{k^2/\Pi + 1}$ we can obtain the equation $1 = (6\lambda/\pi^2)\int_1^\infty \mathrm{d}x\,\sqrt{x^2-1}f(\sqrt{\Pi}x)$. According to the formula,

$$\int_1^\infty \mathrm{d}x\,\sqrt{x^2-1}f(ux) = \frac{2\pi^2T^2}{u^2}\left[\frac{1}{12} - \frac{u}{4\pi T} + \mathcal{O}\left(\frac{u^2}{T^2}\ln\frac{u}{T}\right)\right], \tag{5.68}$$

we obtain

$$\boxed{\Pi = \lambda T^2 - \frac{3T^2\lambda^{3/2}}{\pi} + \cdots.} \tag{5.69}$$

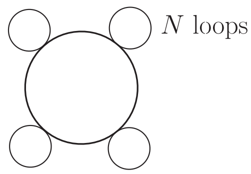
We find that the next-order contribution is proportional to $\lambda^{3/2}$ instead of $\lambda^2$.

**EXERCISE 24**: Plot $\Pi^{1/2}/T$ as a function of $\lambda$ using the exact solution, the solutions at orders $\lambda$ and $\lambda^{3/2}$.

The partition function including interaction could similarly be obtained,

$$\boxed{\ln Z_{\mathrm{int}} = -\langle S_{\mathrm{int}}\rangle_0 + \sum_{N=2}^{\infty}\frac{(-1)^N\langle S_{\mathrm{int}}^N\rangle_{0,\mathrm{c}}}{N!},} \tag{5.70}$$

here "c" abbreviates for "connected", and




$$\begin{aligned}\sum_{N=2}^{\infty}\frac{(-1)^N\langle S_{\mathrm{int}}^N\rangle_{0,\mathrm{c}}}{N!} &= \sum_{N=2}^{\infty}\frac{(-)^N}{N!}6^N2^{N-1}(N-1)!\\ &= \sum_{N=2}^{\infty}\frac{1}{N!}6^N2^{N-1}(N-1)!V\sum_n\int\frac{\mathrm{d}\mathbf{k}}{(2\pi)^3}\frac{(-\Pi_1)^N}{12^N}D_0^N(K) = \frac{V}{2}\sum_n\int\frac{\mathrm{d}\mathbf{k}}{(2\pi)^3}\sum_{N=2}^{\infty}\frac{1}{N}[-\Pi_1D_0(K)]^N\\ &= -\frac{V}{2}\sum_n\int\frac{\mathrm{d}\mathbf{k}}{(2\pi)^3}\{\ln[1+\Pi_1D_0(K)] - \Pi_1D_0(K)\} = -\frac{V}{2}\sum_n\int\frac{\mathrm{d}\mathbf{k}}{(2\pi)^3}\left[\ln\left(1+\frac{\lambda T^2}{\omega_n^2+k^2}\right) - \frac{\lambda T^2}{\omega_n^2+k^2}\right].\end{aligned} \tag{5.71}$$

The pressure is given by combining the zero-temperature contribution and the mode of $n=0$ above, i.e.,

$$\boxed{P \approx \frac{\pi^2T^4}{90} - \frac{\lambda T^4}{48} - \frac{T}{2}\int\frac{\mathrm{d}\mathbf{k}}{(2\pi)^3}\left[\ln\left(1+\frac{\lambda T^2}{k^2}\right) - \frac{\lambda T^2}{k^2}\right] \approx \frac{\pi^2T^4}{90}\left[1 - \frac{15}{8}\frac{\lambda}{\pi^2} + \frac{15}{2}\left(\frac{\lambda}{\pi^2}\right)^{3/2} + \cdots\right].} \tag{5.72}$$

We see again that the next-order contribution to the pressure is $\lambda^{3/2}$.

**EXERCISE 25**: Prove the relation:

$$\int\frac{\mathrm{d}\mathbf{k}}{(2\pi)^3}\left[\ln\left(1+\frac{\lambda T^2}{k^2}\right) - \frac{\lambda T^2}{k^2}\right] = -\frac{\lambda^{3/2}T^3}{6\pi}. \tag{5.73}$$

Discuss how the potential divergence maybe removed.

Perturbatively determining/analyzing different types of correction to a given quantity is a central theme in physical calculations. Finally, we give a few examples and point out certain important ingredients when necessary.

**Example – 1.** The main feature of the estimation on the order of magnitude and approximated perturbative calculations could be clearly demonstrated in some very elementary mathematical problems. For instance, it could be shown when trying to solve the following simple algebraic equation,

$$x^n(t) = \Omega + tx(t)/\Lambda,\quad x(t)\in\mathrm{R}^+,\quad n\in\mathrm{N}^+,\quad n\geq 5,\quad t\geq 0, \tag{5.74}$$

where $t$ and $\Lambda$ are two parameters (e.g., $t$ is the time) with $\Lambda$ a positive constant. As we all know there is no closed formula for the simple algebraic equation if the order of the equation is larger than or equal to five. In this sense we need use either numerical algorithms or approximated methods to investigate the root of the equation like (5.74). If the "time" $t$ is small near zero, the second term on the left hand side of Eq. (5.74) could be treated as a perturbation and in this case we could assume $x(t) \approx x_0[1+\delta(t)] = \Omega^{1/n}[1+\delta(t)]$ with $\delta(t)$ a small correction to the leading order solution "1". Expanding both sides of Eq. (5.74) to order $\delta(t)$, one obtains $\delta(t) = t\Omega^{1/n-1}/n\Lambda$ and then,

$$x(t) \approx \Omega^{1/n}\left(1 + \frac{1}{n\Lambda}\Omega^{1/n-1}t\right). \tag{5.75}$$

The above (approximated) theory will be broken if $t \lesssim n\Lambda\Omega^{1-1/n}$. The approximated theory here is often called the linear perturbation and the basic requirement is that the $t$ should not be larger than $n\Lambda\Omega^{1-1/n}$, e.g., $t \lesssim t_{\max} \approx sn\Lambda\Omega^{1-1/n}, s \ll 1$. Moreover, if one considers the next contribution to the solution, i.e., $x(t) = \Omega^{1/n}(1+\alpha t+\beta t^{\sigma})$, where $\alpha = \Omega^{1/n-1}/n\Lambda$, then after some straightforward calculations, one obtains that $\sigma = 2$ and consequently,

$$x(t) \approx \Omega^{1/n}\left(1+\frac{1}{n\Lambda}\Omega^{1/n-1}t-\frac{n-3}{2n^2\Lambda^2}\Omega^{2/n-2}t^2\right). \tag{5.76}$$

One has that $t \ll n\Lambda\Omega^{1-1/n}$ from the first-order theory. If higher order corrections are taken into consideration, e.g., the second-order contribution appeared in (5.76), the condition for the perturbation theory is obtained as $|(n-3)\delta^2(t)/2| \ll |\delta(t)|$, or equivalently $|(n-3)\delta(t)/2| \ll 1$, or $t \ll 2n\Lambda\Omega^{1-1/n}/(n-3)$. It becomes $t \ll 2\Lambda\Omega^{1-1/n} \sim 2\Lambda\Omega$ if $n$ is large, which is weaker than the criterion $t \ll n\Lambda\Omega^{1-1/n}$, indicating the effective perturbative region shrinks as the order of the expansion increases. The perturbation element (or the small quantity in general) of the Eq. (5.74) is $\delta(t) = \alpha t = \Omega^{1/n-1}t/n\Lambda$, and consequently $x(t) \approx \Omega^{1/n}[1+\delta(t)-(n-3)\delta^2(t)/2]$. It is obvious that it could not be treated as small when the $t$ is large, indicating that either the linear theory or the theory with higher order terms breaks down at large $t$. However, on the other hand, in the limit that the $t$ approaches to infinity, another perturbative scheme for Eq. (5.74) emerges. In that situation, the term $\Omega$ on the right hand side of the equation (5.74) could be safely neglected, leading to $x_{\infty}(t) = (t/\Lambda)^{1/(n-1)}$, and it is called the asymptotic solution (large-$t$) of Eq. (5.74). Assuming that $x(t) \approx x_{\infty}(t)[1+\phi(t)]$ based on the asymptotic solution and the factor $|\phi(t)| \ll 1$, one could obtain,

$$x(t) \approx \left(\frac{t}{\Lambda}\right)^{\frac{1}{n-1}}\left[1+\frac{\Omega}{n-1}\left(\frac{\Lambda}{t}\right)^{\frac{n}{n-1}}\right],\quad \phi(t) = \frac{\Omega}{n-1}\left(\frac{\Lambda}{t}\right)^{\frac{n}{n-1}}, \tag{5.77}$$

with the condition that

$$t \gg t_{\text{asp}} \equiv \Lambda\exp\left(-\frac{n-1}{n}\ln\left(\frac{n-1}{\Omega}\right)\right). \tag{5.78}$$

Moreover, considering that $x(t) \approx x_{\infty}(t)[1+\phi(t)+\mu(t)]$ to even higher order with $\mu(t)$ the contribution smaller than $\phi(t)$, we have

$$x(t) \approx \left(\frac{t}{\Lambda}\right)^{\frac{1}{n-1}}\left[1+\frac{\Omega}{n-1}\left(\frac{\Lambda}{t}\right)^{\frac{n}{n-1}}-\frac{n\Omega^2}{2(n-1)^2}\left(\frac{\Lambda}{t}\right)^{\frac{2n}{n-1}}\right], \tag{5.79}$$

and thus $x(t) \approx x_{\infty}(t)[1+\phi(t)-n\phi^2(t)/2]$, i.e., $\mu(t) = -n\phi^2(t)/2$. The exact solution of the algebraic equation (5.74) could be numerically constructed (e.g., iterative scheme or the Newton's algorithm).

**Example – 2: an effective Hooke's "constant".** Consider the particle moves under a potential having a minimum $x_0$. For motion around $x_0$, the potential acting on the particle could be approximated by expanding the potential $U(x)$ as,

$$U(x) \approx U(x_0)+\dot{U}|_{x=x_0}\delta x+2^{-1}\ddot{U}|_{x=x_0}\delta x^2, \tag{5.80}$$

where $\delta x^n = (x-x_0)^n$, $\dot{U} = \mathrm{d}U/\mathrm{d}x$, and $\ddot{U} = \mathrm{d}^2U/\mathrm{d}x^2$, and since the first-order derivative of the potential at the equilibrium $x_0$ is zero, one obtains

$$\boxed{U_{\text{harm}}(\delta x) = 2^{-1}k^2\delta x^2+\text{const.},\quad k = [U''(x_0)]^{1/2},} \tag{5.81}$$

where the constant is the zero point of the potential (which actually has no fundamental effects on the dynamics processes). The above one is called the harmonic potential, and the solution of which could be obtained exactly. Now, if one tries to study the behavior of the particle far from the equilibrium position $x_0$, the natural treatment is investigating the effects from the high order terms (e.g., the term $\delta x^3$) perturbatively based on the harmonic solution. This is the frequently-used method in physical problems: Firstly obtaining the solution via the simple approximation (here it is given by $U_{\text{harm}}(\delta x)$, the terms like this are often called the non-interacting terms), and then perturbatively computing the high order effects based on the simple solution. The oscillation around the meta-stable states if they exist is also important and the transition from the meta-stable states to the global ground state is an exciting issue in modern field calculations.[1] Consider the extra force $f^{\delta}(x)$ based on Hooke's force in the harmonic system, $\delta x \to x$. In this situation the energy conservation equation becomes $2^{-1}m\dot{x}^2+2^{-1}kx^2+U^{\delta}(x) = 2^{-1}kd_{\max}^2+U^{\delta}(d_{\max})$, where $d_{\max}$ the maximum distance the oscillator could reach, and $U^{\delta}(x)$ is the potential due to the extra force. If the extra potential is homogeneous with order $\alpha$, i.e., $U^{\delta}(\lambda x) = \lambda^{\alpha}U^{\delta}(x)$, the period of the system could be given generally by

$$\boxed{T = 4\sqrt{\frac{m}{k}}\int_0^{\pi/2}\mathrm{d}\eta\left[1+\frac{2U^{\delta}(d_{\max})[1-\sin^{\alpha}\eta]}{kd_{\max}^2\cos^2\eta}\right]^{-1/2}.} \tag{5.82}$$

[1] The tunneling between the true and false vacuum states was investigated in S. Coleman, *Fate of the False Vacuum: Semiclassical Theory*, Phys. Rev. D **15**, 2929 (1977); C. Callan and S. Coleman, *Fate of the False Vacuum. II: First Quantum Corrections*, Phys. Rev. D **16**, 1762 (1977).

In certain situations one can do perturbative calculations based on $\xi=2U^{\delta}(d_{\max})[1-\sin^{\alpha}\eta]/kd_{\max}^2\cos^2\eta$. By taking the extra force as $f^{\delta}(x)=-ax^3(a>0)$, $\xi=(ad_{\max}^2/2k)(1+\sin^2\eta)$, the effective potential is then given by $U_{\text{eff}}(x)=U_{\text{tot}}(x)=2^{-1}kx^2+4^{-1}ax^4$, characterizing the cubic response to the perturbation. However, such effective potential has actually little use since the high order term here still contains the dynamical variable "$x$". One could obtain to order $a^2$ that,

$$T\approx 2\pi\sqrt{\frac{m}{k}}\times\left(1-\frac{3ad_{\max}^2}{8k}+\frac{57a^2d_{\max}^4}{256k^2}\right),\tag{5.83}$$

and the perturbative condition is $\sigma=ad_{\max}^2/k\ll 1$, or equivalently $U^{\delta}(d_{\max})\ll U(d_{\max})/2$. In this formula, if the replacements, $m/k\leftrightarrow\ell/g$, $d_{\max}=\chi_{\max}\ell$ and $a=-mg/6\ell^3$ are made, one immediately obtains the first-order correction coefficient 1/16 in the period of the simple pendulum, namely

$$\boxed{T\approx 2\pi\sqrt{\frac{\ell}{g}}\times\left(1+\frac{1}{16}\chi_{\max}^2+\frac{11}{3072}\chi_{\max}^4+\cdots\right),}\tag{5.84}$$

where $\chi_{\max}$ is the maximum angle of the simple pendulum. However the even higher order corrections could not be obtained simply through (5.83), since the period of the simple pendulum contains higher order corrections from $\sin\chi$. The correction directly from the term $ax^3$ corresponds to the conventional perturbation theories, and the one characterized by the factor $1+16^{-1}\chi_{\max}^2+(11/3072)\chi_{\max}^4+\cdots$ corresponds to the improved perturbations. The fourth-order correction $(11/3072)\chi_{\max}^4$ in the period of the simple pendulum could be decomposed into two terms: the $\chi_{\max}^2$ term and the $\chi_{\max}^4$ term from the interacting energy $E(\chi_{\max})=-mg\ell\cos\chi_{\max}\approx-mg\ell(1-2^{-1}\chi_{\max}^2+24^{-1}\chi_{\max}^4+\cdots)$, or equivalently the terms proportional to $\chi$ and to $\chi^3$ in the force $F(\chi)=-mg\sin\chi\approx-mg(\chi-6^{-1}\chi^3)$. One could obtain the corresponding nonlinear effects simply by considering the $\chi^3$ term based on the harmonic approximation, but the coefficient is 19/3072 (via the formula (5.83)) instead of 11/3072. Improved perturbation indicates that besides the "direct" term — $\chi^3$, the higher order term originated from $\chi$ (e.g., the first term in $\sin\chi\approx\chi-\chi^3/6$) also contributes to the coefficient 11/3072. This latter one is denoted as the "indirect" contribution; in other words, there exists the mode-coupling between the low modes (here characterized by $\chi$) and the high modes (characterized by $\chi^3$), in the sense $\chi^3\leftarrow(\chi^3)^1$ (direct term) + $(\chi^1)^3$ (indirect high order terms). As the index "$n$" appearing in $\chi^n$ becomes large, the mode-coupling pattern will also become more fruitful. We introduce the very basic concept of effective theories. In the case of the force $ax^3$, one could derive an effective Hooke's constant through the period of the system. In particular, according to the general period formula, one has $T=2\pi(m/k_{\text{eff}})^{1/2}=2\pi m^{1/2}k_{\text{eff}}^{-1/2}$ where the effective spring constant is $k_{\text{eff}}\approx k(1+s_1\sigma+s_2\sigma^2)+\mathcal{O}(\sigma^3)$ with $\sigma=ad_{\max}^2/k\ll 1$. In order to reproduce the first two terms as shown in the formula (5.83), i.e., $-3\sigma/8$ and $57\sigma^2/256$, one obtains the two coefficients $s_1=3/4$ and $s_2=-3/128$. The effective Hooke's constant is thus[2]

$$\boxed{k_{\text{eff}}\approx k\times\left(1+\frac{3}{4}\frac{ad_{\max}^2}{k}-\frac{3}{128}\frac{a^2d_{\max}^4}{k^2}\right),}\tag{5.85}$$

and in other applications one could use the effective potential $U_{\text{eff}}(x)=2^{-1}k_{\text{eff}}x^2$. Here the high order effects characterized by the coefficient $a$ appears in the low-order coefficient and the "dynamical" variable "$x$" disappears at the fourth order. However, there exist other approaches to construct the effective parameters, e.g., the Hooke's constant in the presence of the nonlinear force could also be obtained as $\overline{k}_{\text{eff}}=k+ad_{\max}^2/2$ by considering the maximum distance, indicating other mechanisms need to be taken into account in the construction of an effective theory. We have no attempt to introduce/discuss these advanced issues in the present lecture. The effective theories with the high order degrees of freedom integrated out are often called the "low-energy effective theories".

**Example – 3: equation of state of a unitary Fermi gas.** The unitary limit refers to $ak_{\text{F}}\to\infty$ where $a$ is the scattering length and $k_{\text{F}}=p_{\text{F}}$ is the Fermi momentum of the system under consideration. Obviously, the conventional perturbative schemes based on the small quantity $ak_{\text{F}}$ does not apply for the unitary Fermi gas. Conventionally, the equation of state (defined as the energy per particle) for small $ak_{\text{F}}$ is given by

$$\boxed{\text{EOS}\approx\frac{k_{\text{F}}^2}{2m}\left(\frac{3}{5}+\frac{2}{3\pi}k_{\text{F}}a+\frac{4}{35\pi^2}(11-2\ln 2)(k_{\text{F}}a)^2+0.23(k_{\text{F}}a)^3+\cdots\right),}\tag{5.86}$$

here $k_{\text{F}}=(3\pi^2\rho)^{1/3}$ with $\rho$ being the density. The first term here, namely $3k_{\text{F}}^2/10m$ is the free-gas result and $E_{\text{F}}\equiv k_{\text{F}}^2/2m$ is the Fermi energy. We want to analyze $\xi\equiv\mu/E_{\text{F}}$, the Bertsch parameter. Theoretical analysis tells us that besides the limit $ak_{\text{F}}\to 0$, the 4D system is also free. The wave function of a pair of Fermions with opposite spins in dimensions $d$ is $R(r)\sim r^{2-d}$, here $d$ is the distance between the Fermions. When calculating relevant quantities, one needs $\int\mathrm{d}\mathbf{x}|R(r)|^2\sim$

[2] See, B.J. Cai and B.A. Li, *Auxiliary Function Approach for Determining Symmetry Energy at Suprasaturation Densities*, Phys. Rev. C **103**, 054611 (2021), Section III.

$\int \mathrm{d}r r^{d-1} r^{4-2d} \sim \int \mathrm{d}r r^{3-d}$, implying the probability of emergence of such pair near $r = 0$ for $d \geq 4$ is large (singularity). In this sense, we say that the system in 4D is the non-interacting, $\xi = 0$, and one can develop effective theories in 4D and extrapolate the corresponding equation of state to 3D; the idea of Nishida–Son effective theory.[3] The Lagrangian is

$$\boxed{\mathcal{L} = \sum_{\sigma=\uparrow,\downarrow} \psi_\sigma^\dagger \left( i\partial_t + \frac{\nabla^2}{2m} + \mu_\sigma \right) \psi_\sigma + c_0 \psi_\uparrow^\dagger \psi_\downarrow^\dagger \psi_\downarrow \psi_\uparrow = \Psi^\dagger \left( i\partial_t + \frac{\sigma_3 \nabla^2}{2m} + \mu\sigma_3 + \delta\mu \right) \Psi - \frac{1}{c_0} \phi^\dagger \phi + \Psi^\dagger \sigma_+ \Psi \phi + \Psi^\dagger \sigma_- \Psi \phi^\dagger,} \tag{5.87}$$

where $\Psi = (\psi_\uparrow, \psi_\downarrow^\dagger)^\mathrm{T}$ are the two-component Nabmu–Gorkov field, $\sigma_i$ with $i = 1 \sim 3$ are the three Pauli matrices, $\sigma_\pm = (\sigma_1 \pm \sigma_2)/2$, $\mu = (\mu_\uparrow + \mu_\downarrow)/2$, $\delta\mu = (\mu_\uparrow - \mu_\downarrow)/2$, and $c_0$ is the interaction strength between two Fermions. By introducing $\phi = \phi_0 + g\varphi$ where $g = [(8\pi^2\epsilon)^{1/2}/m](m\phi_0/2\pi)^{\epsilon/4}$, $\epsilon = 4 - d$ and $\varphi$ being the fluctuating field and $\phi_0$ the ground state (condensate), one can expand the Lagrangian as $\mathcal{L} = \mathcal{L}_0 + \mathcal{L}_1 + \mathcal{L}_2$:

$$\mathcal{L}_0 = \Psi^\dagger \left( i\partial_t + \frac{\sigma_3 \nabla^2}{2m} + \sigma_+ \phi_0 + \sigma_- \phi_0 \right) \Psi + \varphi^\dagger \left( i\partial_t + \frac{\nabla^2}{4m} \right) \varphi, \tag{5.88}$$

$$\mathcal{L}_1 = g\Psi^\dagger \sigma_+ \Psi \varphi + g\Psi^\dagger \sigma_- \Psi \varphi^\dagger + \mu \Psi^\dagger \sigma_3 \Psi + 2\mu \varphi^\dagger \varphi, \quad \mathcal{L}_2 = -\varphi^\dagger \left( i\partial_t + \frac{\nabla^2}{4m} \right) \varphi - 2\mu \varphi^\dagger \varphi. \tag{5.89}$$

Here, $\mathcal{L}_0$ is the free part and the mass of a Fermion pair is $2m$, $\mathcal{L}_1$ and $\mathcal{L}_2$ define the vertices. The Fermion and the Boson propagators are given by,

$$G(p_0, \mathbf{p}) = \frac{1}{p_0^2 - \varepsilon^2(\mathbf{p}) + i0^+} \begin{pmatrix} p_0 + E(\mathbf{p}) & -\phi_0 \\ -\phi_0 & p_0 - E(\mathbf{p}) \end{pmatrix}; \quad D(p_0, \mathbf{p}) = \left( p_0 - \frac{E(\mathbf{p})}{2} + i0^+ \right)^{-1}, \tag{5.90}$$

where $E(\mathbf{p}) = \mathbf{p}^2/2m$ is the single-particle energy, $\varepsilon(\mathbf{p}) = [E^2(\mathbf{p}) + \phi_0^2]^{1/2}$ is the dispersion relation. Based on this effective theory, one can show that the 1-loop and 2-loop potentials are,

$$U_{\text{eff}}^{(1)}(\phi_0) = \frac{\phi_0}{3} \left[ 1 + \frac{7 - 3(\gamma + \ln 2)}{6} \epsilon \right] \left( \frac{m\phi_0}{2\pi} \right)^{d/2} - \frac{\mu}{\epsilon} \left[ 1 + \frac{1 - 2(\gamma - \ln 2)}{4} \epsilon \right] \left( \frac{m\phi_0}{2\pi} \right)^{d/2}; \quad U_{\text{eff}}^{(2)}(\phi_0) = -C\epsilon\phi_0 \left( \frac{m\phi_0}{2\pi} \right)^{d/2}, \tag{5.91}$$

where $C \approx 0.14424$ is a constant. The total effective potential to this order is then $U_{\text{eff}}(\phi_0) = U_{\text{eff}}^{(1)}(\phi_0) + U_{\text{eff}}^{(2)}(\phi_0)$, the minimum of which gives the condensate field $\phi_0$ as $\phi_0 = (2\mu/\epsilon)[1 + (3C - 1 + \ln 2)\epsilon]$. One sees $\mu$ is really on the order of $\epsilon$. After obtaining the effective potential, one can evaluate the pressure $P = -U_{\text{eff}}(\phi_0)$ and then $\rho = \partial P/\partial\mu$, therefore

$$\boxed{\xi \equiv \frac{\mu}{E_\mathrm{F}} = \frac{1}{2} \epsilon^{3/2} \exp\left( \frac{\epsilon \ln \epsilon}{8 - 2\epsilon} \right) \left[ 1 - \left( 3C - \frac{5}{4}(1 - \ln 2)\epsilon \right) \right] \approx 2^{-1}\epsilon^{3/2} + 16^{-1}\epsilon^{5/2} \ln \epsilon - 0.0246\epsilon^{5/2}.} \tag{5.92}$$

Taking $\epsilon = 1$ gives $\xi \approx 0.475$, which is close to the experimental result $\approx 0.376$.[4] The Nishida–Son theory was later expanded by including higher-order terms in $\epsilon$ and the prediction is even closer to the experimental result.

**Example – 4: corrections to gravitational potential.** The gravitational potential between two masses $m_1$ and $m_2$ with distance $r$ given by $U_\mathrm{G}(r) = -Gm_1m_2/r$ should be modified to be when considering the relevant corrections:[5]

$$\boxed{U_\mathrm{G}^{\text{eff}}(r) \approx -\frac{Gm_1m_2}{r} \left[ 1 - \frac{G(m_1 + m_2)}{rc^2} - \frac{127}{30\pi^2} \frac{G\hbar}{r^2c^3} \right],} \tag{5.93}$$

here the second (third) term is the special-relativity correction characterized by $c$ (quantum correction by $\hbar$).

**EXERCISE 26**: Derive the analytic expressions for the $x(t)$ of Eq. (5.74) to order $\delta^3(t)$ and $\phi^3(t)$. Discuss their applicable conditions; consider the equation by generalizing Eq. (5.74) to be $x^n(t) = \Omega + tx^m(t)/\Lambda$ with $m < n$, develop its approximated solutions.

**EXERCISE 27**: Assume the effective spring constant is $k_{\text{eff}} \approx k(1 + s_1\sigma + s_2\sigma^2 + s_3\sigma^3 + s_4\sigma^4)$, work out the values of $s_3$ and $s_4$.

**EXERCISE 28**: The Coleman–Weinberg potential[6] is the effective potential when including radiative corrections. For a scalar field, the Coleman–Weinberg potential is given by,

$$\boxed{U_{\text{eff}}(\phi_{\text{cl}}) = U(\phi_{\text{cl}}) - \frac{i\hbar}{2} \int \frac{\mathrm{d}^4k}{(2\pi)^4} \ln \left[ 1 - \frac{U''(\phi_{\text{cl}})}{k^2} \right] \to U_{\text{eff}}(\phi_{\text{cl}}) = U(\phi_{\text{cl}}) + \frac{\hbar}{2} \int \frac{\mathrm{d}^4k_\mathrm{E}}{(2\pi)^4} \ln \left[ 1 + \frac{U''(\phi_{\text{cl}})}{k_\mathrm{E}^2} \right],} \tag{5.94}$$

[3] Y. Nishida and D.T. Son, *$\epsilon$ Expansions for a Fermi Gas at Infinite Scattering Length*, Phys. Rev. Lett. **97**, 050403 (2006).

[4] M. Ku et al., *Revealing the Superfluid Lambda Transition in the Universal Thermodynamics of a Unitary Fermi Gas*, Science **335**, 563 (2012).

[5] J. Donoghue, *Leading Quantum Correction to the Newtonian Potential*, Phys. Rev. Lett. **72**, 2996 (1994).

[6] S. Coleman and E. Weinberg, *Radiative Corrections as the Origin of Spontaneous Symmetry Breaking*, Phys. Rev. D **7**, 1888 (1973); S. Coleman, *Aspects of Symmetry*, Cambridge University Press, 1985, Chapter 5; for a recent relevant discussion, see, e.g., A. Andreassen, W. Frost, and M. Schwartz, *Consistent Use of Effective Potentials*, Phys. Rev. D **91**, 016009 (2015).

where the second expression follows from using $k^0 = ik_0^{\mathrm{E}}$ and $\mathbf{k} = \mathbf{k}_{\mathrm{E}}$, and therefore $\mathrm{d}^4k = i\mathrm{d}^4k_{\mathrm{E}}$ as well as $k^2 = -k_{\mathrm{E}}^2$. Obviously, (5.94) is a semi-classical expansion based on $\hbar$. Adopting $U(\phi) = 2^{-1}\mu^2\phi^2 + \lambda\phi^4/4!$, considering the counter-terms $B\phi_{\mathrm{cl}}^2 + C\phi_{\mathrm{cl}}^4$ in the effective potential and the renormalization conditions $\mathrm{d}^2U_{\mathrm{eff}}(\phi_{\mathrm{cl}})/\mathrm{d}\phi_{\mathrm{cl}}^2|_{\phi_{\mathrm{cl}}=0} = 0$ together with $\mathrm{d}^4U_{\mathrm{eff}}(\phi_{\mathrm{cl}})/\mathrm{d}\phi_{\mathrm{cl}}^4|_{\phi_{\mathrm{cl}}=M} = \lambda(M)$ to show

$$U_{\mathrm{eff}}(\phi_{\mathrm{cl}}) = \frac{1}{24}\lambda(M)\phi_{\mathrm{cl}}^4 + \frac{\lambda^2(M)\phi_{\mathrm{cl}}^4}{256\pi^2}\left[\ln\left(\frac{\phi_{\mathrm{cl}}^2}{M^2}\right) - \frac{25}{6}\right] + \mathcal{O}[\lambda^2(M)]. \tag{5.95}$$

For the (0+1)-dimensional problem, show that $U_{\mathrm{eff}}(\phi_{\mathrm{cl}}) = U(\phi_{\mathrm{cl}}) + 2^{-1}\hbar\mu[1 + \lambda\phi_{\mathrm{cl}}^2/2\mu^2]^{1/2}$. Obviously, $U_{\mathrm{eff}}(0)$ is the zero-point energy.

## F Linear Perturbations, Retarded Response and Correlation Functions

RELEVANT REFERENCE:

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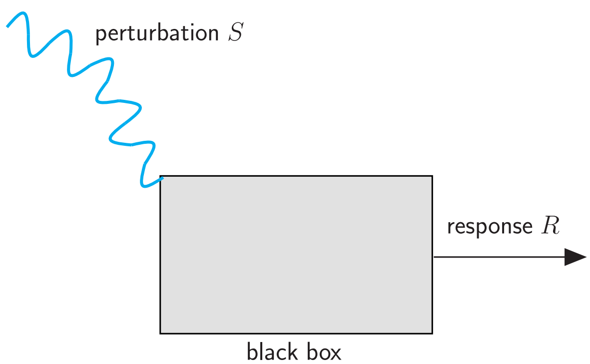


Fig. G: The black box executes a response $R$ when a perturbation $S$ is applied on it.

When we perturb a system (nuclear matter, solid, etc.), generally treated as a black box, the system would response correspondingly. Let us execute a perturbation $S$ on the black box, then the latter generally responses characterized by $R$. If the perturbation is not quite strong (weak), the response $R$ is expected to be proportional to $S$, i.e.,

$$R = \beta S, \tag{6.1}$$

where $\beta$ is the corresponding proportionality coefficient. An elementary example is the Hooke's force applied on a spring with coefficient $k$, i.e., $F = -kx$ where $x$ is the distance from the equilibrium position. By measuring the linear response $F$ with a distance $x$, one can straightforwardly determine Hooke's constant $k$, therefore linear responses could be measured. To develop a theory for a given system, it is therefore extremely important to calculate various linear responses from the theory, because these results are usually the easiest to check by experiment. Consider a 1D harmonic oscillator with Hamiltonian $H_0 = p^2/2m + 2^{-1}mW^2x^2$ and a dipole interaction $\delta H = -e\mathrm{E}x$, here E is the electric field. The induced dipole momentum is given by $d = \langle\overline{n}|ex|\overline{n}\rangle$, here $|\overline{n}\rangle$ is the ground state of $H_0 + \delta H$. To the first order of perturbation theory, $|\overline{n}\rangle$ is given by

$$|\overline{n}\rangle = |0\rangle + \sum_{n=1,2,\cdots}|n\rangle\frac{\langle n|\delta H|0\rangle}{E_0 - E_n}, \tag{6.2}$$

here $|n\rangle$ is the ground state of $H_0$. The dipole momentum is then obtained as ($\chi$ is the susceptibility)

$$d = -2\mathrm{E}\sum_{n=1,2,\cdots}\frac{\langle 0|ex|n\rangle\langle n|ex|0\rangle}{E_0 - E_n} = \frac{2e^2}{W}\langle 0|x^2|0\rangle\mathrm{E} \equiv \chi\mathrm{E}. \tag{6.3}$$

The above result can be expressed in terms of correlation functions. To understand the general relationship between linear response and correlation functions, we consider a general quantum system described by $H_0$. We then turn the perturbation on and off slowly and calculate the linear response using standard time-dependent perturbation theory. After including a time-dependent perturbation $f(t)\mathcal{O}_1$, the total Hamiltonian is given as

$$H(t) = H_0 + f(t)\mathcal{O}_1, \tag{6.4}$$

Here, $f(t) = 0$ for $t$ less than a starting time. To obtain the response of an $H_0$ eigenstate $|\psi_n\rangle$ under the perturbation $f(t)\mathcal{O}_1$, we start with $|\psi_n\rangle$ at $t_{-\infty} = -\infty$. Then, at a finite time $t$,

$$\boxed{|\psi_n(t)\rangle = \mathrm{T}\exp\left(-i\int_{-\infty}^{t}\mathrm{d}t' H(t')\right)|\psi_n\rangle,} \tag{6.5}$$

where T is the time-ordering operator which puts the latest operator on the leftest side. We can expand $|\psi_n(t)\rangle$ to first order in $\mathcal{O}_1$ as,

$$|\psi_n(t)\rangle = \exp\left(-i\int_{-\infty}^{t} \mathrm{d}t' H_0\right)|\psi_n\rangle + \delta|\psi_n(t)\rangle, \tag{6.6}$$

where

$$\delta|\psi_n(t)\rangle = -i\int_{-\infty}^{t} \mathrm{d}t' f(t') e^{-iH_0(t-t')}\mathcal{O}_1 e^{-iH_0(t'-t_{-\infty})}|\psi_n\rangle = -i\int_{-\infty}^{t} \mathrm{d}t' f(t') e^{-iH_0(t-t_{-\infty})}\underbrace{e^{iH_0(t'-t_{-\infty})}\mathcal{O}_1 e^{-iH_0(t'-t_{-\infty})}}_{\mathcal{O}_1(t')}|\psi_n\rangle \tag{6.7}$$

To obtain the change of the physical quantity $\mathcal{O}_2$ in the response to the perturbation $f(t)\mathcal{O}_1$, we calculate

$$\boxed{\begin{aligned}\delta\langle\psi_n(t)|\mathcal{O}_2|\psi_n(t)\rangle &\equiv \langle\psi_n(t)|\mathcal{O}_2|\psi_n(t)\rangle - \langle\psi_n|e^{iH_0(t-t_{-\infty})}\mathcal{O}_2 e^{-iH_0(t-t_{-\infty}}|\psi_n\rangle \\ &\approx -i\int_{-\infty}^{t}\mathrm{d}t' f(t')\langle\psi_n|[\mathcal{O}_2(t),\mathcal{O}_1(t')]|\psi_n\rangle + \cdots \\ &= \int_{-\infty}^{\infty}\mathrm{d}t' D(t,t') f(t'),\end{aligned}} \tag{6.8}$$

where $D(t,t')$ is the response function defined by

$$\boxed{iD(t,t') = \Theta(t-t')\langle\psi_n|[\mathcal{O}_2(t),\mathcal{O}_1(t')]|\psi_n\rangle.} \tag{6.9}$$

At zero temperature, one can take $|\psi_n\rangle$ to be the ground state $|\psi_0\rangle$. If $H_0$ is time independent, then $D(t,t')$ would be a function of $t-t'$ only, which could be written as $D(t-t')$. The response $\delta\langle\mathcal{O}_2\rangle$ for the ground state is given by

$$\boxed{\delta\langle\mathcal{O}_2\rangle = \int_{-\infty}^{\infty}\mathrm{d}t' D(t-t') f(t').} \tag{6.10}$$

The factor $\Theta(t-t')$ in $D(t-t')$ tells only when $t>t'$ it is nonzero, implying the retarded nature.

We now use the formula (6.10) to deal with the dipole momentum of the above harmonic oscillator. In this case, $-e\mathrm{E}$ plays the role of $f(t)$ and $\mathcal{O}_2 = \mathcal{O}_1 = ex$, so the response function is

$$D(t-t') = -i\Theta(t-t')\langle 0|[x(t),x(t')]|0\rangle = -2\langle 0|x^2|0\rangle\Theta(t-t')\sin W(t-t'). \tag{6.11}$$

Moreover, we should turn on the electric field slowly in the sense that $\mathrm{E}(t) = \mathrm{E}e^{-\epsilon|t|}$, therefore

$$d = \int_{-\infty}^{\infty}\mathrm{d}t' e^2 D(t-t')e^{\epsilon t'}(-\mathrm{E}) = -e^2\int \mathrm{d}t D(t)\mathrm{E} = \frac{2e^2}{W}\langle 0|x^2|0\rangle\mathrm{E}. \tag{6.12}$$

If we introduce the Fourier transform of $D(t)$ as

$$\boxed{D(\omega) = \int \mathrm{d}t D(t)e^{i\omega t},} \tag{6.13}$$

then $d = -e^2 D(\omega=0)\mathrm{E}$. We see that the linear response of an electric dipole to an electric field is related to the correlation of the dipole operator $ex$. In fact, all of the other linear responses have a similar structure, namely the coefficients of the linear responses can be calculated from the correlation functions of appropriate operators, e.g., the conductivity can be calculated from the correlation function of the current operators. A few examples:

(a) Density: the corresponding operator is $\psi^\dagger\psi$ and the response function is charge susceptibility.

(b) Spin density, then the operator and response function are $\psi_a^\dagger\vec{\sigma}_{ab}\psi_b$ and spin susceptibility, respectively.

(c) For current density, we have $(e/m)\psi^\dagger(-i\nabla - e\mathbf{A})\psi$ for the operator and the response function is conductivity.

The retarded response function (6.9) could be generalized to finite temperature,

$$\boxed{iD_\mathrm{R}(t-t') = \sum_n \Theta(t-t')\langle\psi_n|[\mathcal{O}(t),\mathcal{O}(t')]|\psi_n\rangle\frac{e^{-\beta E_n}}{Z} \equiv \Theta(t-t')\langle[\mathcal{O}(t),\mathcal{O}(t')]\rangle,} \tag{6.14}$$

where $Z$ is the partition function and subscript "R" is added, (6.14) is often called the Kubo Formula. In the remaining of this section we take $\mathcal{O}_2 = \mathcal{O}_1 = \mathcal{O}$, and $\langle\cdots\rangle$ indicates the ensemble average. Then a similar formula as (6.10) could be written out,

$$\boxed{\langle \mathcal{O}(t)\rangle = \langle \mathcal{O}\rangle + \int \mathrm{d}t D(t-t')f(t').} \tag{6.15}$$

We define the correlation $C(t-t')$ as

$$\boxed{C(t-t') = \langle \mathcal{O}(t)\mathcal{O}(t')\rangle = \int \frac{\mathrm{d}\omega}{2\pi} e^{-i\omega(t-t')}C(\omega).} \tag{6.16}$$

Therefore $C(t) = \langle \mathcal{O}(t)\mathcal{O}(0)\rangle$ represents the fluctuation of the operator $\mathcal{O}$ after time $t$.

Inserting a complete set of energy eigenstates $|n\rangle$ of $H$ with energy $E_n$ and considering gives

$$\langle n|\mathcal{O}(t)|m\rangle = \langle n|e^{iHt}\mathcal{O}e^{-iHt}|m\rangle = e^{-it(E_m-E_n)}\langle n|\mathcal{O}|m\rangle, \tag{6.17}$$

we can write the correlation function as

$$C(t-t') = \sum_{n,m} \frac{e^{-\beta E_n}}{Z}\langle n|\mathcal{O}(t)|m\rangle\langle m|\mathcal{O}(t')|n\rangle = \sum_{n,m} \frac{e^{-\beta E_n}}{Z}|\langle n|\mathcal{O}|m\rangle|^2 e^{-i(E_m-E_n)(t-t')}. \tag{6.18}$$

The frequency-dependent correlation function can be written

$$\boxed{C(\omega) = \int \mathrm{d}t e^{i\omega t}C(t) = \sum_{n,m} \frac{e^{-\beta E_n}}{Z}|\langle n|\mathcal{O}|m\rangle|^2 2\pi\delta(E_m - E_n - \omega).} \tag{6.19}$$

Using the similar technique, we can write out the spectral decomposition of the retarded response function,

$$iD_{\mathrm{R}}(t-t') = \Theta(t-t')\sum_{n,m}\frac{e^{-\beta E_n} - e^{-\beta E_m}}{Z}|\langle n|\mathcal{O}|m\rangle|^2 e^{-i(E_m-E_n)(t-t')}, \tag{6.20}$$

equivalently, we have

$$\boxed{D_{\mathrm{R}}(t) = -i\Theta(t)\sum_{n,m}\frac{e^{-\beta E_n} - e^{-\beta E_m}}{Z}|\langle n|\mathcal{O}|m\rangle|^2 e^{-it(E_m-E_n)}.} \tag{6.21}$$

By introducing the spectral function (the meaning of $\overline{D}$ will become clear later)

$$\overline{D}(\omega) = -\pi\left(1 - e^{-\beta\omega}\right)\sum_{n,m}\frac{e^{-\beta E_n}}{Z}|\langle n|\mathcal{O}|m\rangle|^2\delta(\omega - (E_m - E_n)), \tag{6.22}$$

the retarded response function becomes,

$$D_{\mathrm{R}}(t) = i\int \frac{\mathrm{d}\omega}{\pi} e^{-i\omega t}\Theta(t)\overline{D}(\omega). \tag{6.23}$$

Fourier transforming this result, one could read off,

$$D_{\mathrm{R}}(\omega) = \int \frac{\mathrm{d}\omega'}{\pi}\frac{\overline{D}(\omega')}{\omega' - \omega - i\epsilon}. \tag{6.24}$$

This is know as a Kramers–Kronig relation, which could be used to extend the response function into the complex plane by writing

$$\boxed{D(z) = \int \frac{\mathrm{d}\omega'}{\pi}\frac{\overline{D}(\omega')}{\omega' - z}.} \tag{6.25}$$

We call this the dynamical susceptibility. If one can do an experiment to determine how much the system absorbs at all frequencies, then from this information one can determine the response of the system at zero frequency, which is known as the thermodynamic sum rule. When we evaluate $D(z)$ just above the real axis, we get the retarded response function $D_{\mathrm{R}} = D(\omega + i\epsilon)$. The upper half-plans is therefore the analytic extension of $D_{\mathrm{R}}(\omega)$. When considering about the lower half-plane, the concept of advanced response function emerges such that $D_{\mathrm{A}}(\omega) = D(\omega - i\epsilon)$. From the definition of $D(z)$, we could find that its poles are located exclusively along the real axis at $z = \omega'$, so that $D(z)$ is analytic everywhere except the real axis. Substituting the basic relation

$$\frac{1}{\omega - \omega' \pm i\epsilon} = \mathcal{P}\left(\frac{1}{\omega - \omega'}\right) \mp \pi i\delta(\omega - \omega'), \tag{6.26}$$

where $\mathcal{P}$ denotes the principal part, we can obtain

$$D(\omega \pm i\epsilon) = \int \frac{\mathrm{d}\omega'}{\pi}\mathcal{P}\left(\frac{1}{\omega'-\omega}\right)\overline{D}(\omega') \pm i\overline{D}(\omega). \tag{6.27}$$

So that the real part of $D(z)$ is continuous across the real axis, but the dissipative imaginary part has a discontinuity:

$$\overline{D}(\omega) \equiv \mathrm{Im}\, D(\omega+i\epsilon) = \frac{1}{2i}[D(\omega+i\epsilon)-D(\omega-i\epsilon)] = \frac{i}{2}[D(\omega-i\epsilon)-D(\omega+i\epsilon)] \tag{6.28}$$

We often introduce the notations $D(\omega) = \mathrm{Re}D(\omega) + i\mathrm{Im}D(\omega) \equiv D'(\omega) + iD''(\omega)$. The imaginary part $D''(\omega)$ is called the dissipative or absorptive part of the response function. It is also known as the spectral function, which will become apparent after we discuss Green's function theories in the next section.

**EXERCISE 29**: Show the real (imaginary) part of the response function is even (odd), and argue the imaginary part is dissipative.
**EXERCISE 30**: Show that the Kramers–Kronig relation could also be written in the following form,

$$\boxed{\mathrm{Re}\, D(\omega) = \mathcal{P}\int_{-\infty}^{+\infty}\frac{\mathrm{d}\omega'}{\pi}\frac{\mathrm{Im}\, D(\omega')}{\omega-\omega}, \quad \mathrm{Im}\, D(\omega) = -\mathcal{P}\int_{-\infty}^{+\infty}\frac{\mathrm{d}\omega'}{\pi}\frac{\mathrm{Re}\, D(\omega')}{\omega-\omega},} \tag{6.29}$$

implying the two parts are not independent.

Combining (6.19) and (6.21) leads to

$$\boxed{C(\omega) = -2[1+n_{\mathrm{B}}(\omega)]\,\mathrm{Im}\, D(\omega), \quad n_{\mathrm{B}} = \frac{1}{e^{\beta\omega}-1}.} \tag{6.30}$$

This is the famous fluctuation–dissipation theorem, $n_{\mathrm{B}}$ is the Bose distribution. We see explicitly two terms contribute to the fluctuations, namely the $n_{\mathrm{B}}(\omega)$ factor is due to thermal effects while the "1" can be thought of as due to inherently quantum fluctuations. As usual, the classical limit occurs for high temperatures with $\beta\omega \ll 1$ where $n_{\mathrm{B}} \approx k_{\mathrm{B}}T/\omega$. In this regime, the fluctuation–dissipation theorem reduces to its classical counterpart $C(\omega) = -2k_{\mathrm{B}}T\mathrm{Im}D(\omega)/\omega$.

The fluctuation–dissipation theorem could be established in a classical harmonic oscillator. Suppose that thermal fluctuations give rise to a random force, acting on the oscillator according to the equation of motion,

$$\boxed{m\ddot{x} + mW^2x + \gamma\dot{x} = F(t),} \tag{6.31}$$

here $\gamma > 0$ is the damping coefficient. Fourier transforming both sides and considering $\int x^{(n)}e^{i\omega t}\mathrm{d}t = (-i\omega)^n x(\omega)$, we may obtain the equation of motion in $\omega$ space,

$$x(\omega) = \chi(\omega)F(\omega), \quad \chi(\omega) = \frac{1}{m(W^2-\omega^2)-i\omega\gamma}. \tag{6.32}$$

Here $\chi(\omega)$ is the response function or susceptibility to the external force. The imaginary part of the susceptibility is,

$$\boxed{\chi''(\omega) = \frac{\omega\gamma}{m^2(W^2-\omega^2)^2+\omega^2\gamma^2} = |\chi(\omega)|^2\omega\gamma,} \tag{6.33}$$

which governs the dissipation (since it is proportional to $\gamma$). Over long time periods, one expects that the two-point correlation function to be purely a function of the time difference, namely $S(t,t') = \langle x(t)x(t)'\rangle = \langle x(t-t')x(0)\rangle$. The power spectrum of fluctuations $\langle |x(\omega)|^2\rangle$ is defined as the Fourier transform of $\langle x(t)x(0)\rangle$, therefore its inverse transform gives

$$\boxed{\langle x(t)x(t')\rangle = \int \frac{\mathrm{d}\omega}{2\pi}e^{-i\omega(t-t')}\langle |x(\omega)|^2\rangle.} \tag{6.34}$$

Under thermal equilibrium, the equipartition equilibrium theorem tells us that $2^{-1}mW^2\langle x^2\rangle = k_{\mathrm{B}}T/2$, or equivalently

$$\langle x^2\rangle = \int \frac{\mathrm{d}\omega}{2\pi}\langle |x(\omega)|^2\rangle = \int \frac{\mathrm{d}\omega}{2\pi}|\chi(\omega)|^2\langle |F(\omega)|^2\rangle = \frac{k_{\mathrm{B}}T}{mW^2}. \tag{6.35}$$

Since the integration over $\omega$ is very sharply peaked around $|\omega| = W$, one can replace $\langle |F(\omega)|^2\rangle \to \langle |F(W)|^2\rangle$ when doing the relevant calculations. Replacing $|\chi(\omega)|^2$ with $\chi''(\omega)/\omega\gamma$, we then have

$$\frac{k_{\mathrm{B}}T}{mW^2} = \frac{\langle |F(W)|^2\rangle}{2\gamma}\int \frac{\mathrm{d}\omega}{\pi}\frac{\chi''(\omega)}{\omega} = \frac{\langle |F(W)|^2\rangle}{2\gamma m W^2}. \tag{6.36}$$

So the spectrum of the fluctuations is determined by the damping force (viscosity $\gamma$) as,

$$\boxed{\langle |F(W)|^2\rangle = 2\gamma k_{\mathrm{B}} T.} \tag{6.37}$$

If we assume that the noise spectrum depends only on the properties of the damping medium in which the oscillator is embedded, and not fundamentally on the properties of the oscillator itself, (6.37) is expected to hold for any frequency $W$. In this sense, we conclude that the power spectrum of the force is a flat function of frequency. This consequently implies that in thermal equilibrium the force coupling the system to the environment is a source of white noise of an amplitude which depends on the viscosity of the medium,

$$\boxed{\langle F(t)F(t')\rangle = \int \frac{\mathrm{d}\omega}{2\pi} e^{-i\omega(t-t')}\langle |F(\omega)|^2\rangle = 2\gamma k_{\mathrm{B}} T\delta(t-t').} \tag{6.38}$$

The noise spectrum of fluctuations is given by

$$\boxed{S(\omega) \equiv \langle |x(\omega)|^2\rangle = |\chi(\omega)|^2\langle |F(\omega)|^2\rangle = \langle |F(\omega)|^2\rangle \frac{\chi''(\omega)}{\omega\gamma} = \frac{2k_{\mathrm{B}}T}{\omega}\chi''(\omega),} \tag{6.39}$$

or inversely

$$\boxed{\overbrace{S(t) = \langle x(t)x(0)\rangle}^{\text{fluctuations}} = 2k_{\mathrm{B}}T\int \frac{\mathrm{d}\omega}{2\pi} e^{-i\omega t} \underbrace{\frac{\chi''(\omega)}{\omega}}_{\text{dissipation}},} \tag{6.40}$$

which says that fluctuations in a classical harmonic oscillator are directly related to the dissipative response function via the fluctuation–dissipation theorem. This form of fluctuation–dissipation theorem is consistent with (6.30) at high temperatures (using $S \leftrightarrow -C$ for the notation consistency).

**EXERCISE 31**: Solve the damped harmonic oscillator (with $F(t) = 0$) under appropriate initial conditions; use the imaginary part $\chi''(\omega)$ to obtain the real part $\chi'(\omega)$ via the Kramers–Kronig relation; define $\tan\Phi(\omega) = \chi''(\omega)/\chi'(\omega)$, what's the meaning of $\Phi$?

**EXERCISE 32**: Show that in hydrodynamic problems, the response function takes the form of

$$D_{\text{sound}}(\omega) \sim \frac{1}{\omega^2 - v_{\mathrm{s}}^2 k^2}, \tag{6.41}$$

where $v_{\mathrm{s}}$ is the speed of sound. Argue how the viscosity could be obtained from the response function.

**EXERCISE 33**: Define the advanced response function, $iD_{\mathrm{A}}(t-t') = \Theta(t'-t)\langle[\mathcal{O}(t), \mathcal{O}(t')]\rangle$, show that

$$D_{\mathrm{A}}(\omega) = \int \frac{\mathrm{d}\omega'}{\pi}\frac{\mathrm{Im}\, D(\omega')}{\omega' - \omega + i\epsilon}. \tag{6.42}$$

What's the physical meaning of this response function?

Finally, we derive the imaginary-time response function. The partition function in the presence of a perturbation of the form $f(\tau)\mathcal{O}$ is evaluated as,

$$Z = Z_0\left\langle \mathrm{T}\exp\left(-\int_0^\beta \mathrm{d}\tau f(\tau)\mathcal{O}(\tau)\right)\right\rangle. \tag{6.43}$$

The expectation value of $\mathcal{O}(\tau)$ is then given by to linear order,

$$\langle \mathcal{O}(\tau)\rangle = \frac{\delta \ln Z}{\delta f(\tau)} = \frac{\left\langle \mathrm{T}\mathcal{O}(\tau)\exp\left(-\int_0^\beta \mathrm{d}\tau' f(\tau')\mathcal{O}(\tau')\right)\right\rangle}{\left\langle \mathrm{T}\exp\left(-\int_0^\beta \mathrm{d}\tau' f(\tau')\mathcal{O}(\tau')\right)\right\rangle} \approx \langle \mathcal{O}\rangle - \int_0^\beta \mathrm{d}\tau' \left[\left\langle \mathrm{T}\mathcal{O}(\tau)\mathcal{O}(\tau')\right\rangle - \langle \mathcal{O}\rangle^2\right] f(\tau'). \tag{6.44}$$

Therefore,

$$\boxed{\langle \mathcal{O}(\tau)\rangle = \langle \mathcal{O}\rangle - \int_0^\beta \mathrm{d}\tau' D^{(\mathrm{im})}(\tau-\tau')f(\tau'),\ \ D^{(\mathrm{im})}(\tau-\tau') = \left\langle \mathrm{T}\mathcal{O}(\tau)\mathcal{O}(\tau')\right\rangle - \langle \mathcal{O}\rangle^2.} \tag{6.45}$$

Using the similar technique as in the real-time situation, one can show

$$\boxed{D^{(\mathrm{im})}(i\omega_n) = \int \frac{\mathrm{d}\omega}{\pi}\frac{1}{\omega - i\omega_n}\mathrm{Im}\, D^{(\mathrm{im})}(\omega),} \tag{6.46}$$

where $\omega_n$ is the Matsubara frequency. Compared with (6.25), we find that (6.46) is nothing more than the dynamical susceptibility $D(z)$, evaluated at $z = i\omega_n$. In other words, $D^{(\mathrm{im})}(i\omega_n)$ is the unique analytic extension of $D(\omega)$ into the complex plane. It therefore provides a procedure to calculate response functions, namely writing $D^{\mathrm{im}}(i\omega_n)$ in the form (6.46), and using this to read off $D''(\omega)$ which in turn reconstructs the dynamical response function via (6.25).

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