UNIVERSITÄT KÖLN, INSTITUT FÜR THEORETISCHE PHYSIK

Vorlesung: Quanten-Phasen-Übergänge

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Contents

1 Introduction

1.1 What is a QPT?

1.2 Experimental Examples of QPTs

2 Quantum Statistical Mechanics

2.1 Generalities

2.2 Example: The 1d Josephson Junction Array

2.3 Dynamics and Thermodynamics

3 The Vicinity of the Quantum Critical Point: Scaling

3.1 Dynamic Scaling

3.2 Finite-Size Scaling

3.3 Classical-Quantum Crossover, Dephasing

4 Quantum Hall Systems

4.1 Generalities

4.2 Temperature and Frequency Scaling

4.3 Current Scaling

4.4 Universal Resistivities (Amplitudes)

4.5 Problems

5 The Feynman path-integral

5.1 Real-time path-integral

Schrödinger says that

$$\langle q', t' | q, t \rangle = \langle q' | \mathrm{e}^{-\frac{i}{\hbar}\hat{H}(t'-t)} | q \rangle \ . \tag{5.1}$$

For small times, one can work with the linearized version, for which one needs:

$$\langle q' | \hat{H} | q \rangle \ . \tag{5.2}$$

We specify

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{q}) \tag{5.3}$$

$$[\hat{p}, \hat{q}] = \frac{\hbar}{i} \ . \tag{5.4}$$

Let us calculate (5.2)

$$\langle q' | \hat{H} | q \rangle = \int \frac{\mathrm{d}p}{2\pi\hbar} \, \langle q' | p \rangle \, \langle p | \hat{H} | q \rangle = \int \frac{\mathrm{d}p}{2\pi\hbar} \, \mathrm{e}^{\frac{i}{\hbar} p (q'-q)} \, H(p,q) \ , \tag{5.5}$$

where $H(p,q)$ is the classical Hamilton-function

$$H(p,q) = \frac{p^2}{2m} + V(q) \ , \tag{5.6}$$

and

$$\langle q | p \rangle = \mathrm{e}^{ipq/\hbar} \ , \qquad \int \frac{\mathrm{d}p}{2\pi\hbar} \, |p\rangle\langle p| = 1 \ . \tag{5.7}$$

Writing $\langle q', t' | q, t \rangle$ as the product of transition amplitudes for small time-slices and integrating over the intermediate steps, we have with the usual notation

$$\langle q', t' | q, t \rangle = \int \mathcal{D}[q] \, \mathcal{D}[p] \, \mathrm{e}^{\frac{i}{\hbar} \int_t^{t'} p(t)\dot{q}(t) - H(p(t), q(t))} \ . \tag{5.8}$$

Performing the integral over the p's, which can always be done as long as the action is not more than quadratic in p, the result is (up to some normalization N)

$$\langle q', t' | q, t \rangle = \frac{1}{N} \int \mathcal{D}[q] \, \mathrm{e}^{\frac{i}{\hbar} \int_t^{t'} L(q(t), \dot{q}(t))} \ , \tag{5.9}$$

where $L(q, \dot{q})$ is defined by (saddle-points for quadratic actions are exact!)

$$L(q, \dot{q}) = p\dot{q} - H(p,q) \Big|_{\dot{q} = \partial H(p,q)/\partial p} \ . \tag{5.10}$$

We recognize this as the usual Legendre transfrom, relating the Hamilton-function $H(p,q)$ to the Lagrange-function $L(q,\dot{q})$. Equation (5.9) is the famous Feynman path-integral, introduced in [1].

A direct derivation without introducing the field p can also be given. See section about the Laplace-DeGennes-transform where this is done in details for the Wick-rotated version.

Question: Which formulation is the fundamental one when $H(p,q)$ is not quadratic in q?
Answer: The formulation with $H(p,q)$. Our considerations with $H(p,q)$ are completely general, wherease when working with $L(q,\dot{q})$, one has to make assumptions on the form of the kinetic term.

5.2 Imaginary time path-integral: The partition function

We now use the normalizations as in section 5.1, to calculate a path-integral representation for the partition function. This might not seem the most natural normalization to calculate $\mathrm{tr}(\mathrm{e}^{-\beta \hat{H}})$, since the latter does not contain $\hbar$; however these are the appropriate normalizations in order to establish the connection between dynamics and thermodynamics.

We calculate the partition-function, thus

$$\mathcal{Z} = \mathrm{tr}(\mathrm{e}^{-\beta \hat{H}}) \; . \tag{5.11}$$

Using the Trotta formula to decompose $\beta \hat{H}$ as $\beta \hat{H} = \frac{1}{\hbar} \int_0^{\beta\hbar} \mathrm{d}\tau \, \hat{H}$, and using (5.5) we get

$$\mathcal{Z} = \int \mathcal{D}[q] \, \mathcal{D}[p] \, \mathrm{e}^{\frac{1}{\hbar} \int_0^{\beta\hbar} \mathrm{d}\tau (ip(\tau)\dot{q}(\tau) - H(p(\tau), q(\tau)))} \; . \tag{5.12}$$

In difference to (5.10), the weight-function is now the Euclidean action $S_{\mathrm{E}}[q, \dot{q}]$, given by the saddle-point

$$0 = \frac{\partial}{\partial p} \Big(ip\dot{q} - H(p,q) \Big) \tag{5.13}$$

as

$$L_{\mathrm{E}}(q, \dot{q}) = -L\left(q, i\dot{q}\right) \;, \quad S_{\mathrm{E}} = \int_0^{\beta\hbar} \mathrm{d}\tau \, L_{\mathrm{E}}(q(\tau), \dot{q}(\tau))) \; . \tag{5.14}$$

The sign-convention in the definition of S_{E} is such that

$$\mathcal{Z} = \int \mathcal{D}[q] \mathrm{e}^{-\frac{1}{\hbar} S_{\mathrm{E}}} \; . \tag{5.15}$$

Also note that observables can be calculated, by inserting them into the path-integral. The path-integral naturally orders observables by their time (earlier to the right).

5.3 The action for more general Hamiltonians and commutation-relations

We now want to construct the path-integral for more general Hamilton-operators and more general commutation-relations. Suppose that we have a quantum field theory given by (K_{xy} is supposed to be real):

$$\mathcal{H}(\hat{\phi}_x, \hat{\Pi}_x) \;, \qquad \left[\hat{\Pi}_x, \hat{\phi}_y \right] = \frac{\hbar}{i} K_{xy} \;, \qquad \left[\hat{\phi}_x, \hat{\phi}_y \right] = 0 \;, \qquad \left[\hat{\Pi}_x, \hat{\Pi}_y \right] = 0 \tag{5.16}$$

This is sufficient to construct the path-integral, as one can see from the following: First, we construct the ϕ-representation of the operator $\hat{\Pi}_x$:

$$\hat{\Pi}_x = \frac{\hbar}{i} \int_y K_{xy} \frac{\delta}{\delta \phi_y} \;, \tag{5.17}$$

which is checked by remarking that it reproduces the commutation-relation (5.16). To construct the path-integral, we need the basis-change from ϕ to Π, which from $\left(\Pi_x - \frac{\hbar}{i} \int_y K_{xy} \frac{\delta}{\delta \phi_y} \right) \langle \phi | \Pi \rangle = 0$ is inferred to be

$$\langle \phi | \Pi \rangle = \det \left[K_{xy} \right]^{-\frac{1}{2}} \mathrm{e}^{\frac{i}{\hbar} \int_x \int_y \Pi_x K^{-1}_{xy} \phi_y} \; . \tag{5.18}$$

The normalization (often dropped) is checked from

$$\int \mathcal{D}\left[\Pi\right] \langle \phi | \Pi \rangle \langle \Pi | \phi' \rangle = \det \left[K_{xy} \right]^{-1} \int \mathcal{D}\left[\Pi\right] \mathrm{e}^{\frac{i}{\hbar} \int_x \int_y (\phi_x - \phi'_x) K^{-1}_{xy} \Pi_y} = \int \mathcal{D}\left[\Pi'\right] \mathrm{e}^{\frac{i}{\hbar} \int_x \int_y (\phi_x - \phi'_x) \Pi'_x} \;, \tag{5.19}$$

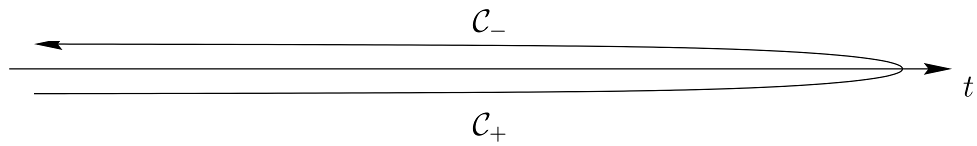

Figure 1: The Keldysh contour

which is the δ-distribution for ϕ.

This gives the generalized path-integral

$$\langle \phi_{x,t} | \phi_{0,0} \rangle = \int \mathcal{D}\left[\phi\right] \mathcal{D}\left[\Pi\right] \mathrm{e}^{\frac{i}{\hbar}\mathcal{S}} \tag{5.20}$$

$$\mathcal{S} = \int_0^t \mathrm{d}t \int_x \Pi_x K_{xy}^{-1} \dot{\phi}_y - \mathcal{H}(\phi, \Pi) \tag{5.21}$$

Since from the action, we can calculate *all* observables, this also leads to the following
Theorem: A Quantum theory is given by its classical Hamilton-function, e.g. as a function of coordinates (or fields) and conjugate momenta, and their commutation relations.

6 The Keldysh-formalism

Here, I construct some formulas as what is known as the "Keldysh-formalism".

Denote for any contour $\mathcal{C}$

$$S_{\mathcal{C}} := \int_{\mathcal{C}} \mathrm{d}t \, L(q(t), \dot{q}(t)) \ . \tag{6.1}$$

We also use

$$S_+ := S_{\mathcal{C}_+} \ , \qquad S_- := S_{\mathcal{C}_-} \tag{6.2}$$

$$U_+ = \mathrm{e}^{i/\hbar S_+} \ , \qquad U_- = \mathrm{e}^{i/\hbar S_-} \ . \tag{6.3}$$

Let us call the time-variable on the lower path t_+ (since it goes into positive direction) and that on the upper path t_-. Also $q_+ = q(t_+)$ a.s.o. Thus

$$S_+ = \int \mathrm{d}t \, m \frac{\dot{q}_+^2}{2} - V(q_+) \tag{6.4}$$

$$S_- = \int \mathrm{d}t \, m \frac{\dot{q}_-^2}{2} - V(q_-) \ . \tag{6.5}$$

Now introduce coordinates in the center-of-mass system.

$$q_\pm := q \pm \breve{q} \tag{6.6}$$

$$q = \frac{1}{2}\left(q_+ + q_-\right) \tag{6.7}$$

$$\breve{q} = \frac{1}{2}\left(q_+ - q_-\right) \ . \tag{6.8}$$

Then

$$S_{\mathcal{C}} := S_+ - S_- = \int \mathrm{d}t \left(L_+ - L_-\right) , \tag{6.9}$$

since path $\mathcal{C}_-$ has the opposite direction as path $\mathcal{C}_+$.

$$\begin{aligned} S_{\mathcal{C}} &= \int_{t_i}^{t_f} \mathrm{d}t\, m \left(\frac{\dot{q}_+^2}{2} - \frac{\dot{q}_-^2}{2} \right) - V(q_+) + V(q_-) \\ &= \int_{t_i}^{t_f} \mathrm{d}t\, 2m\, \dot{\breve{q}}\dot{q} - V(q + \breve{q}) + V(q - \breve{q}) \\ &= -\int_{t_i}^{t_f} \mathrm{d}t\, 2m\, \breve{q} \frac{\mathrm{d}^2}{\mathrm{d}t^2} q + V(q + \breve{q}) - V(q - \breve{q}) \ , \end{aligned} \tag{6.10}$$

where in the last partial integration boundary terms are neglected.

One should be able to calculate correlation-functions by inserting fields into the contour-integral, say all in $\mathcal{C}_+$. This would give ($q_1 := q(t_1)$)

$$\begin{aligned} \langle \mathcal{O}_1 \mathcal{O}_2 \rangle &= \int \mathcal{D}[q]\, \mathcal{D}[\breve{q}]\, \mathcal{O}_1(q_1 + \breve{q}_1) \mathcal{O}_2(q_2 + \breve{q}_2)\, \mathrm{e}^{\frac{i}{\hbar} S} \\ &= \int \mathcal{D}[q]\, \mathcal{D}[\breve{q}]\, \mathcal{O}_1(q_1 + \breve{q}_1) \mathcal{O}_2(q_2 + \breve{q}_2) \\ &\qquad \times \exp\left[-\frac{i}{\hbar} \int_{t_i}^{t_f} \mathrm{d}t\, 2m\, \breve{q} \frac{\mathrm{d}^2}{\mathrm{d}t^2} q + V(q + \breve{q}) - V(q - \breve{q}) \right] \ . \end{aligned} \tag{6.11}$$

Response-functions should be constructed by looking at an observable $\mathcal{O}_2$ reacting to a change in the potential (a force) $\delta\mathcal{L}(q, \dot{q}) = \delta(t - t_1)\mathcal{O}_1(q)$ at time t_1. (Note that making a change in $\mathcal{L}$ is equivalent to making a change in $-\mathcal{H}$. Since the force is $-\nabla V$, this will for $\mathcal{O}_1 = q$ be the response to a uniform force, with the correct sign.) Also note that this perturbation appears in both parts of the Keldysh-integral. Its linear response is

$$\begin{aligned} &\frac{i}{\hbar} \int \mathcal{D}[q]\, \mathcal{D}[\breve{q}]\ \left[\mathcal{O}_1(q_1 + \breve{q}_1) - \mathcal{O}_1(q_1 - \breve{q}_1) \right] \mathcal{O}_2(q_2 + \breve{q}_2) \\ &\qquad \times \exp\left[-\frac{i}{\hbar} \int_{t_i}^{t_f} \mathrm{d}t\, 2m\, \breve{q} \frac{\mathrm{d}^2}{\mathrm{d}t^2} q + V(q + \breve{q}) - V(q - \breve{q}) \right] \ . \end{aligned} \tag{6.12}$$

Choosing $\mathcal{O}_1 = \mathcal{O}_2 = q$, this gives

$$R_{qq} = \frac{2i}{\hbar} \left\langle \breve{q}_1 (q_2 + \breve{q}_2) \right\rangle \ . \tag{6.13}$$

6.1 A change in variables and the classical limit (MSR-action)

Staring at the path-integral

$$\begin{aligned} &\int \mathcal{D}[q]\, \mathcal{D}[\breve{q}]\, \mathcal{O}_1(q_1 + \breve{q}_1) \mathcal{O}_2(q_2 + \breve{q}_2) \\ &\qquad \times \exp\left[-\frac{i}{\hbar} \int_{t_i}^{t_f} \mathrm{d}t\, 2m\, \breve{q} \frac{\mathrm{d}^2}{\mathrm{d}t^2} q + V(q + \breve{q}) - V(q - \breve{q}) \right] \ , \end{aligned} \tag{6.14}$$

we define a new field $\tilde{q}$

$$\boxed{\tilde{q} := \frac{2i}{\hbar} \breve{q} \equiv \frac{i}{\hbar} (q_+ - q_-)} \tag{6.15}$$

In this new field, (6.14) becomes (the integration over $\tilde{q}$ running from $-i\infty$ to $i\infty$)

$$\int \mathcal{D}[q]\,\mathcal{D}[\tilde{q}]\,\mathcal{O}_1(q_1+\frac{\hbar}{2i}\tilde{q}_1)\mathcal{O}_2(q_2+\frac{\hbar}{2i}\tilde{q}_2)$$
$$\times\exp\left[-\int_{t_i}^{t_f}\mathrm{d}t\, m\,\tilde{q}\frac{\mathrm{d}^2}{\mathrm{d}t^2}q+\frac{i}{\hbar}V(q+\frac{\hbar}{2i}\tilde{q})-\frac{i}{\hbar}V(q-\frac{\hbar}{2i}\tilde{q})\right]\,, \tag{6.16}$$

Using the convention of $\mathrm{e}^{-\mathcal{S}}$, we have

$$-\mathcal{S}\equiv\frac{i}{\hbar}S \tag{6.17}$$

relating the new Keldysh-action to the real action.

$$\mathcal{S}=\int_{t_i}^{t_f}\mathrm{d}t\, m\,\tilde{q}\frac{\mathrm{d}^2}{\mathrm{d}t^2}q+\frac{i}{\hbar}V(q+\frac{\hbar}{2i}\tilde{q})-\frac{i}{\hbar}V(q-\frac{\hbar}{2i}\tilde{q}) \tag{6.18}$$

The classical limit is obtained upon taking $\hbar\to 0$. The action is then expanded as

$$\mathcal{S}=\int_{t_i}^{tf}\mathrm{d}t\,\tilde{q}\left(m\frac{\mathrm{d}^2}{\mathrm{d}t^2}q+V'(q)-\frac{\tilde{q}^2\hbar^2}{24}V'''(q)+\dots\right)\,, \tag{6.19}$$

which is just the MSR-action + higher order terms in $\hbar$.

6.2 Boundary-conditions and the Feynman-Vernon-influence function

We want to study something like (note that E'_n need not be equivalent to $\langle n|\mathcal{H}|n\rangle$, but can be taken from an initial Hamiltonian $\mathcal{H}'$.)

$$\frac{1}{\mathcal{Z}}\sum_n\langle n|U_-\mathcal{O}U_+|n\rangle\mathrm{e}^{-\beta E'_n}\,. \tag{6.20}$$

This can be written as the *Feynman-Vernon-influence-function* [2]

$$\int_{q_1}\int_{q_2}\frac{\langle q_1|\mathrm{e}^{-\beta\mathcal{H}'}|q_2\rangle}{\mathcal{Z}}\langle q_2|U_-\mathcal{O}U_+|q_1\rangle\,, \tag{6.21}$$

where

$$\mathcal{Z}:=\mathrm{tr}\left(\mathrm{e}^{-\beta\mathcal{H}'}\right)\,. \tag{6.22}$$

Let us now calculate some observables. For the moment, we prepare the system with a different Hamiltonian $\mathcal{H}'$ than the time-evoluting one $\mathcal{H}$. This condition will be dropped later.

$$\langle q_+(t)q_+(t')\rangle=\frac{1}{\mathcal{Z}}\mathrm{tr}\left(\mathrm{e}^{-\beta\mathcal{H}'}T^+q(t)q(t')\right) \tag{6.23}$$

On the l.h.s. stand expectation values in the path integral, whereas on the r.h.s. expectation values in the operator formalism.

$$q(t):=\mathrm{e}^{i\mathcal{H}t}\,q\,\mathrm{e}^{-i\mathcal{H}t} \tag{6.24}$$

and T^+ the time ordering operator, putting larger times to the left. T^- is the anti-time ordering opertor, thus analogously

$$\langle q_-(t)q_-(t')\rangle=\frac{1}{\mathcal{Z}}\mathrm{tr}\left(\mathrm{e}^{-\beta\mathcal{H}'}T^-q(t)q(t')\right)\,. \tag{6.25}$$

Further, since q_+ is always earlier on the contour,

$$\langle q_+(t)q_-(t')\rangle = \frac{1}{\mathcal{Z}}\mathrm{tr}\left(\mathrm{e}^{-\beta\mathcal{H}'}q(t)q(t')\right) \ . \tag{6.26}$$

Therefore, using our earlier definitions in (6.6) ff. we obtain with the time-ordering operator on the Keldysh-contour $\mathcal{C}$

$$\langle q(t)q(t')\rangle = \frac{1}{4\mathcal{Z}}\mathrm{tr}\left(\mathrm{e}^{-\beta\mathcal{H}'}T_{\mathcal{C}}\left\{(q_+(t)+q_-(t))(q_+(t')+q_-(t'))\right\}\right) \ . \tag{6.27}$$

Observing that e.g. for $t<t'$, $q_+(t)$ is always first in the trace, and $q_-(t')$ always last, we get with (6.24)

$$\begin{aligned}\langle q(t)q(t')\rangle &= \frac{1}{2\mathcal{Z}}\,\mathrm{tr}\left(\mathrm{e}^{-\beta\mathcal{H}'}\left\{q(t)q(t')+q(t')q(t)\right\}\right)\\ &= \frac{1}{2\mathcal{Z}}\,\mathrm{tr}\left(\mathrm{e}^{-\beta\mathcal{H}'}\left\{q(t),q(t')\right\}\right) \ .\end{aligned} \tag{6.28}$$

Next is

$$\begin{aligned}\langle q(t)\breve{q}(t')\rangle &= \frac{1}{4\mathcal{Z}}\mathrm{tr}\left(\mathrm{e}^{-\beta\mathcal{H}'}T_{\mathcal{C}}\left[(q_+(t)+q_-(t))(q_+(t')-q_-(t'))\right]\right)\\ &= \frac{1}{4\mathcal{Z}}\mathrm{tr}\left(\mathrm{e}^{-\beta\mathcal{H}'}T_{\mathcal{C}}\left[q_+(t)q_+(t')-q_+(t)q_-(t')+q_-(t)q_+(t')-q_-(t)q_-(t')\right]\right)\\ &= \Theta(t-t')\frac{1}{2\mathcal{Z}}\mathrm{tr}\left(\mathrm{e}^{-\beta\mathcal{H}'}\left[q(t),q(t')\right]\right) \ .\end{aligned} \tag{6.29}$$

Last:

$$\begin{aligned}\langle \breve{q}(t)\breve{q}(t')\rangle &= \frac{1}{4\mathcal{Z}}\mathrm{tr}\left(\mathrm{e}^{-\beta\mathcal{H}'}T_{\mathcal{C}}\left[(q_+(t)-q_-(t))(q_+(t')-q_-(t'))\right]\right)\\ &= \frac{1}{4\mathcal{Z}}\mathrm{tr}\left(\mathrm{e}^{-\beta\mathcal{H}'}T_{\mathcal{C}}\left[q_+(t)q_+(t')+q_-(t)q_-(t')-q_+(t)q_-(t')-q_-(t)q_+(t')\right]\right)\\ &= 0 \ .\end{aligned} \tag{6.30}$$

These formulas are similar to MSR. The Green-function (response-function) is causal, i.e. *retarded*. Note that from (6.29), and due to (6.30) the response-function is

$$R(t-t') := \frac{\delta\left\langle q(t)\right\rangle}{\delta L(t')} = \frac{2i}{\hbar}\left\langle \breve{q}(t')q(t)\right\rangle \tag{6.31}$$

Using the above and the definition (6.15) of $\tilde{q}$, we arrive at the important formula

$$\boxed{R(t,t') = \langle q(t)\tilde{q}(t')\rangle = \Theta(t-t')\frac{i}{\hbar\mathcal{Z}}\mathrm{tr}\left(\mathrm{e}^{-\beta\mathcal{H}'}\left[q(t),q(t')\right]\right)} \ . \tag{6.32}$$

The correlation function is for comparison

$$\boxed{C(t,t') = \langle q(t)q(t')\rangle = \frac{1}{2\mathcal{Z}}\,\mathrm{tr}\left(\mathrm{e}^{-\beta\mathcal{H}'}\left\{q(t),q(t')\right\}\right) \ .} \tag{6.33}$$

6.3 FDT

Let us now derive the FDT. To do so, we need $\mathcal{H}' = \mathcal{H}$. (At least they have to commute. Otherwise $\mathrm{e}^{-\beta\mathcal{H}'}$ is not diagonal in the same basis as $\mathrm{e}^{it\mathcal{H}/\hbar}$. Here we suppose, they are equal.) We use

$$\mathrm{tr}\left(\mathrm{e}^{-\beta\mathcal{H}}q(t)q(t')\right) = \sum_{n,m} \langle n|\, \mathrm{e}^{\frac{i}{\hbar}\mathcal{H}t} q \mathrm{e}^{-\frac{i}{\hbar}\mathcal{H}t} \,|m\rangle \, \langle m|\, \mathrm{e}^{\frac{i}{\hbar}\mathcal{H}t'} q \mathrm{e}^{-\frac{i}{\hbar}\mathcal{H}t'} \,|n\rangle \, \mathrm{e}^{-\beta E_n} \tag{6.34}$$

to insert a complete set of energy-eigenstates into both (6.28) and (6.29):

$$\langle q(t)q(t')\rangle = \frac{1}{2\mathcal{Z}} \sum_{n,m} |\langle n|q|m\rangle|^2 \, \mathrm{e}^{-\beta E_n} \left(\mathrm{e}^{i(t-t')(E_n-E_m)/\hbar} + \mathrm{e}^{-i(t-t')(E_n-E_m)/\hbar}\right) \tag{6.35}$$

$$\langle q(t)\breve{q}(t')\rangle = \Theta(t-t')\frac{1}{2\mathcal{Z}} \sum_{n,m} |\langle n|q|m\rangle|^2 \, \mathrm{e}^{-\beta E_n} \left(\mathrm{e}^{i(t-t')(E_n-E_m)/\hbar} - \mathrm{e}^{-i(t-t')(E_n-E_m)/\hbar}\right) \ . \tag{6.36}$$

Both functions are (for $t > t'$) real and imaginary part of $\frac{1}{2\mathcal{Z}}\sum_{n,m} |\langle n|q|m\rangle|^2 \, \mathrm{e}^{-\beta E_n} \mathrm{e}^{i(t-t')(E_n-E_m)/\hbar}$. We now go to frequency-space.

$$\begin{aligned}
\langle q(\omega)q(-\omega)\rangle &= \int_{-\infty}^{\infty} \mathrm{d}t\, \mathrm{e}^{-i\omega t} \, \langle q(t)q(0)\rangle \\
&= \int_{-\infty}^{\infty} \mathrm{d}t\, \mathrm{e}^{-i\omega t} \frac{1}{2\mathcal{Z}} \sum_{n,m} |\langle n|q|m\rangle|^2 \, \mathrm{e}^{-\beta E_n} \left(\mathrm{e}^{it(E_n-E_m)/\hbar} + \mathrm{e}^{-it(E_n-E_m)/\hbar}\right) \\
&= \int_{-\infty}^{\infty} \mathrm{d}t\, \mathrm{e}^{-i\omega t} \frac{1}{2\mathcal{Z}} \sum_{n,m} |\langle n|q|m\rangle|^2 \left(\mathrm{e}^{-\beta E_n} + \mathrm{e}^{-\beta E_m}\right) \mathrm{e}^{it(E_n-E_m)/\hbar} \\
&= \frac{1}{2\mathcal{Z}} \sum_{n,m} |\langle n|q|m\rangle|^2 \left(\mathrm{e}^{-\beta E_n} + \mathrm{e}^{-\beta E_m}\right) 2\pi\delta(\omega + (E_m - E_n)/\hbar) \\
&= (1+\mathrm{e}^{-\beta\omega\hbar})\frac{1}{2\mathcal{Z}} \sum_{n,m} |\langle n|q|m\rangle|^2 \, \mathrm{e}^{-\beta E_n} 2\pi\delta(\omega + (E_m - E_n)/\hbar) \ .
\end{aligned} \tag{6.37}$$

The response function is (adding $-i\delta$ to ω to ensure convergence; also note the integral starts at $t = 0$ due to the Θ-function in (6.36).)

$$\begin{aligned}
&\langle q(\omega)\breve{q}(\omega)\rangle \\
&= \int_{0}^{\infty} \mathrm{d}t\, \mathrm{e}^{-i\omega t - \delta t} \, \langle q(t)\breve{q}(0)\rangle \\
&= \int_{0}^{\infty} \mathrm{d}t\, \mathrm{e}^{-i\omega t - \delta t} \frac{1}{2\mathcal{Z}} \sum_{n,m} |\langle n|q|m\rangle|^2 \, \mathrm{e}^{-\beta E_n} \left(\mathrm{e}^{it(E_n-E_m)/\hbar} - \mathrm{e}^{-it(E_n-E_m)/\hbar}\right) \\
&= \int_{0}^{\infty} \mathrm{d}t\, \mathrm{e}^{-i\omega t - \delta t} \frac{1}{2\mathcal{Z}} \sum_{n,m} |\langle n|q|m\rangle|^2 \left(\mathrm{e}^{-\beta E_n} - \mathrm{e}^{-\beta E_m}\right) \mathrm{e}^{it(E_n-E_m)/\hbar} \\
&= \frac{1}{2\mathcal{Z}} \sum_{n,m} |\langle n|q|m\rangle|^2 \left(\mathrm{e}^{-\beta E_n} - \mathrm{e}^{-\beta E_m}\right) \frac{1}{\delta + i\omega + i(E_m - E_n)/\hbar} \\
&= \frac{1}{2\mathcal{Z}} \sum_{n,m} |\langle n|q|m\rangle|^2 \left(\mathrm{e}^{-\beta E_n} - \mathrm{e}^{-\beta E_m}\right) \left[\mathcal{P}\frac{-i}{\omega + (E_m - E_n)/\hbar} + \pi\delta(\omega + (E_m - E_n)/\hbar)\right] \ .
\end{aligned} \tag{6.38}$$

The real part of that is

$$(1-\mathrm{e}^{-\beta\hbar\omega})\frac{1}{2\mathcal{Z}}\sum_{n,m}|\langle n|q|m\rangle|^2\,\mathrm{e}^{-\beta E_n}\pi\delta(\omega+(E_m-E_n)/\hbar)\ . \tag{6.39}$$

The FDT is

$$\langle q(\omega)q(-\omega)\rangle = 2\coth\left(\frac{\beta\hbar\omega}{2}\right)\Im\,\langle q(\omega)i\breve{q}(-\omega)\rangle \tag{6.40}$$

In terms of the physical correlation $C(\omega)$ and response-function $R(\omega)$, this is

$$\boxed{C(\omega)=\hbar\coth\left(\frac{\beta\hbar\omega}{2}\right)\Im\,R(\omega)}\ . \tag{6.41}$$

In the limit of $\hbar\to 0$, this reduces to

$$C(\omega)\xrightarrow{\hbar\to 0}\frac{2}{\omega\beta}\Im\,R(\omega)\ . \tag{6.42}$$

As a function of the time-difference, we state without proof the result

$$R(t)=\frac{\beta}{2}\Theta(t)\frac{\mathrm{d}}{\mathrm{d}t}C(t)\ . \tag{6.43}$$

6.4 The Matsubara-relation

Let us recall that (6.29) gives (if $\mathcal{H}=\mathcal{H}'$)

$$\langle q(t)\breve{q}(0)\rangle=\Theta(t)\frac{1}{2\mathcal{Z}}\mathrm{tr}\left(\mathrm{e}^{-\beta\mathcal{H}}\left[q(t),q(0)\right]\right)\ , \tag{6.44}$$

and from the second to last line of (6.38) its Fourier-transform is

$$\langle q(\omega)\breve{q}(\omega)\rangle=\frac{1}{2\mathcal{Z}}\sum_{n,m}|\langle n|q|m\rangle|^2\left(\mathrm{e}^{-\beta E_n}-\mathrm{e}^{-\beta E_m}\right)\frac{1}{\delta+i\omega+i(E_n-E_m)/\hbar}\ . \tag{6.45}$$

We now define the imaginary time correlation-function (also called Matsubara-function) for $0\le\tau\le\beta\hbar$ (which can be continued analytically to $\tau\in\mathbb{R}$ giving a $\beta\hbar$-periodic function.)

$$U(\tau):=\frac{1}{\mathcal{Z}}\mathrm{tr}\left(\mathrm{e}^{-(\beta-\tau/\hbar)\mathcal{H}}q\,\mathrm{e}^{-(\tau/\hbar)\mathcal{H}}\,q\right)\ . \tag{6.46}$$

Its Fourier-transform is defined for

$$\omega_n:=\frac{2\pi n}{\beta\hbar}\ ,\ n\in\mathbb{Z} \tag{6.47}$$

as

$$U(\omega_n):=\int_0^{\beta\hbar}\mathrm{d}\tau\,\mathrm{e}^{-i\omega_n\tau}U(\tau)\ . \tag{6.48}$$

The inverse is

$$U(\tau)=\frac{1}{\beta\hbar}\sum_n\mathrm{e}^{i\omega_n\tau}U(\omega_n)\ . \tag{6.49}$$

Similar to what we have done to derive (6.45), see (6.38), we now insert two complete sets of eigenfunctions of $\mathcal{H}$

$$
\begin{aligned}
U(\omega_n) &= \frac{1}{\mathcal{Z}} \int_0^{\beta\hbar} \mathrm{d}\tau\, \mathrm{e}^{-i\omega_n \tau} \mathrm{tr}\left(\mathrm{e}^{-(\beta-\tau/\hbar)\mathcal{H}} q\, \mathrm{e}^{-\tau\mathcal{H}/\hbar}\, q \right) \\
&= \frac{1}{\mathcal{Z}} \int_0^{\beta\hbar} \mathrm{d}\tau\, \mathrm{e}^{-i\omega_n \tau} \sum_{n,m} |\langle n|q|m\rangle|^2 \mathrm{e}^{-\beta E_m - \tau(E_n - E_m)/\hbar} \\
&= \frac{1}{\mathcal{Z}} \sum_{n,m} |\langle n|q|m\rangle|^2 \left(\mathrm{e}^{-\beta E_n} - \mathrm{e}^{-\beta E_m} \right) \frac{1}{-i\omega_n + (E_n - E_m)/\hbar} \\
&= \frac{i}{\mathcal{Z}} \sum_{n,m} |\langle n|q|m\rangle|^2 \left(\mathrm{e}^{-\beta E_n} - \mathrm{e}^{-\beta E_m} \right) \frac{1}{\omega_n + i(E_n - E_m)/\hbar} \,.
\end{aligned} \tag{6.50}
$$

Note that by going from line 2 to 3, we have needed that ω_n is quantised by (6.47); the factors of $\mathrm{e}^{-\beta E_n}$ and $\mathrm{e}^{-\beta E_m}$ are the boundary values of the integration. Comparing (6.45) and (6.50), we arrive at

$$
\langle q(\omega)\breve{q}(\omega)\rangle = \frac{1}{2i} U(\omega_n{=}i\omega + \delta) \,. \tag{6.51}
$$

The physical response-function is $R(\omega) = \langle q(\omega)\tilde{q}(\omega)\rangle$ such that

$$
\boxed{R(\omega) = \frac{1}{\hbar} U(\omega_n{=}i\omega + \delta)} \,. \tag{6.52}
$$

The correlation-function can then be obtained from the FDT (6.41) as

$$
C(\omega) = \coth\left(\frac{\beta\hbar\omega}{2}\right) \Im U(\omega_n{=}i\omega + \delta) \,. \tag{6.53}
$$

One can also relate the response-function in the time-variable. Using (6.32) and the definition of $U(\tau)$ in (6.46), we can write

$$
\boxed{R(t) = \Theta(t) \frac{i}{\hbar} \left[U(\tau \to it + \delta) - U(\tau \to it - \delta) \right]} \,, \tag{6.54}
$$

where δ serves to give the time-ordering. Equivalently, the correlation-function is from (6.33) obtained as

$$
\boxed{C(t) = \frac{1}{2} \left[U(\tau \to it + \delta) + U(\tau \to it - \delta) \right]} \,, \tag{6.55}
$$

6.5 Free theory

Study the quadratic action (note that the weight is $\mathrm{e}^{-\mathcal{S}}$)

$$
\mathcal{S} = \int_{x,t} \tilde{u} \left(m\partial_t^2 - \Delta \right) u + \frac{i}{\hbar} V\left(u + \tfrac{\hbar}{2i}\tilde{u} \right) - \frac{i}{\hbar} V\left(u(x,t) - \tfrac{\hbar}{2i}\tilde{u} \right) \tag{6.56}
$$

where $V(u) = \kappa u^2$. This gives

$$
\mathcal{S} = \int_{x,t} \tilde{u} \left(m\partial_t^2 - \Delta + \kappa \right) u \tag{6.57}
$$

Two paths can be taken to calculate the response-function. First in analogy to MSR, we have directly

$$R(\omega, k) = \frac{1}{k^2 + \kappa - m\omega^2} \ , \tag{6.58}$$

where a priori it is not clear, which is the way to shift the poles from the axis. However, this could be obtained by demanding (6.58) to be causal (retarded). The other method is to use the Matsubara technique. The problem is, that one first has to construct the path-integral. Following the line of arguments that led from (6.4) to (6.18) and (6.19), we have for the Lagrange-function

$$L = \int_x \frac{m}{2}\left(\frac{\mathrm{d}}{\mathrm{d}t}u\right)^2 - \frac{1}{2}(\nabla u)^2 - \frac{\kappa}{2}u^2 \tag{6.59}$$

Continuing to Euclidean time, we have as Euclidean action the immediate generalization of (5.14):

$$S_{\mathrm{E}} = \int_0^{\beta\hbar} \mathrm{d}\tau \int_x \frac{m}{2}\left(\frac{\mathrm{d}}{\mathrm{d}\tau}u\right)^2 + \frac{1}{2}(\nabla u)^2 + \frac{\kappa}{2}u^2 \tag{6.60}$$

We know how to calculate the correlation-function of this model, which is the Matsubara-function ($\omega_n \in \frac{2\pi}{\beta\hbar}\mathbb{N}$):

$$U(k, \omega_n) = \langle u(k, \omega_n) u(-k, -\omega_n) \rangle = \frac{\hbar}{k^2 + m\omega_n^2/\hbar^2 + \kappa} \ , \tag{6.61}$$

where the $\hbar$ comes from $\mathrm{e}^{-S_{\mathrm{E}}/\hbar}$. Using relation (6.52), this gives for the response-function

$$R(k, \omega) = \frac{1}{\hbar} U(k, \hbar(i\omega + \delta)) = \frac{1}{k^2 - m(\omega - i\delta)^2 + \kappa} \tag{6.62}$$

We can check, that this is causal:

$$\int \frac{\mathrm{d}\omega}{2\pi} \mathrm{e}^{i\omega t} R(k, \omega) = \Theta(t) \frac{\sin\left(\frac{t\sqrt{k^2+\kappa}}{\sqrt{m}}\right)}{\sqrt{m}\sqrt{k^2 + \kappa}} \tag{6.63}$$

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