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Dissipative Quantum Phase Transition in Cold Atomic Gases

Dissipativer Quanten-Phasenübergang in kalten
Gasen

Diploma Thesis written by
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Statutory Declaration:

I declare that I have written this thesis independently and have not used any other sources or aids than those referenced in this work.

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Abstract

We study the influence of a dissipative environment on a quantum mechanical system. The considered system is a particle in a periodic potential at zero temperature, which tunnels between neighboring minima. The environment is represented by one-dimensional Bose-Einstein condensates overlaying each minimum of the potential. We derive the microscopic Hamiltonian of the system and map it onto the spin-boson Hamiltonian describing a dissipative two-state system. Thus we obtain the physical parameters like the coupling strength between the particle and the environment. In the path integral formulation of statistical mechanics we derive the effective partition function and rewrite it in the Coulomb gas formulation of interacting charges. Then we apply the renormalization group method to the partition function and derive the flow equation which yields the critical coupling strength that marks the quantum dissipative phase transition.

Contents

1	Introduction	7
2	Basic Concepts	9
2.1	Dissipative quantum mechanical system	9
2.1.1	Caldeira-Leggett model	9
2.1.2	Dissipative two state system	10
2.2	Construction of the path integral	13
2.3	Statistical mechanics	15
2.4	Path integral and statistical mechanics	16
2.5	Bose Einstein condensation (BEC)	18
2.6	Bogoliubov theory	19
2.7	Tight binding (TB) model and charge picture	21
3	Mapping between the microscopic and the spin-boson-system	25
3.1	The microscopic system	25
3.2	Derivation of the microscopic Hamiltonian describing the double well	26
3.3	Mapping between the Hamiltonians describing the double well	28
3.3.1	Mapping between the TSS-Hamiltonians	28
3.3.2	Environment mapping	28
3.3.3	Interaction mapping	29
3.4	Microscopic lattice	37
3.4.1	Derivation of the microscopic Hamiltonian describing the lattice	37
3.4.2	Physical parameters of the microscopic lattice	39
4	Effective action	41
4.1	Density matrix of the reduced system	41
4.1.1	Derivation of the influence action	42
4.2	Effective action in the TB model	46
4.2.1	Influence action in the charge picture	46
4.3	Interaction Lagrangian and influence action for the microscopic system	49
4.3.1	Double well and delta double well	50
4.4	Influence action for the delta system in the charge picture	52
4.4.1	Charge condition	52
4.4.2	Interactions for the path of each well	53

4.4.3	Exact expression for the influence action of the delta-system	54
4.4.4	Simplifying the sum over the interacting charges for the SB-system	56
4.4.5	Simplifying the sum over the interacting charges for the delta-system . . .	58
5	Quantum phase transition	61
5.1	Renormalization group and quantum phase transition	61
5.2	Partition function in the TB model	61
5.3	Renormalization of the partition function	62
5.3.1	Rescaling of the partition function describing the new problem	63
5.3.2	Flow equation and critical value	65
6	Summary and outlook	69
	Bibliography	71
	Acknowledgments	73

Introduction

A real quantum mechanical system can not be considered as isolated, since there is always a dissipative environment present. Therefore the ideal description of standard quantum mechanics is an idealization of the physical system. One must expect that the physical behavior of the system is altered or at least affected by the coupling to an environment. Thus a quantum dissipative description would provide important physical information. There are several concepts of implementing dissipation into the quantum mechanical framework, like introducing a time-dependent Hamiltonian. A very convenient and successful concept is to couple the system of interest to a heat bath of harmonic oscillators and to consider the global system, which preserves the total energy. In 1966 P. Ullersma [1] was one of the first to apply this model to quantum mechanics. A few years later A.O. Caldeira and A.J. Leggett [2, 3, 4] considered a dissipative two-state-system, also named spin-boson-system, and studied the influence of dissipation on the quantum mechanical tunneling process. In 1983 A. Schmid [5] and S.A. Bulgadaev [6], expanded the system and considered a particle tunneling between the neighboring minima of a periodic potential. Obviously the physical behavior of the particle is sensitive to the coupling strength between the system and the environment. The effect of the environment is similar to a quantum mechanical measurement, that determines the quantum mechanical state of the system. In the case of weak coupling the coupling strength is small and the system is nearly unaffected by the environment. This phase is characterized as diffusive. If the coupling strength is increased, the influence of the environment becomes strong. In this case the particle is monitored by the environment, as if measurements were permanently taken. Hence the particle shows no longer diffusive behavior, but becomes localized at a critical coupling strength. Thus, the system exhibited a dissipative quantum phase transition.

In this thesis we are going to investigate how the influence of the environment changes, when the coupling between the particle and the environment is altered. This can be achieved by considering a different physical setup. In our system the environment is represented by one-dimensional Bose-Einstein-condensates, also named bose tubes, that overlay each minimum of the potential. In chapter 3 we derive the microscopic Hamiltonian and map it onto the spin-boson-Hamiltonian in order to determine the physical parameters of our system. In chapter 4 we elaborate the difference between the microscopic system and the spin-boson-system on the basis of the path integral formulation of statistical mechanics. This formulation leads to an effective description of the theory which does not explicitly depend on the environment. As shown by Schmid [5] for the spin-boson system, the effective partition function can be formulated in the

charge picture, also named Coulomb gas model. In this model the influence of the environment is expressed by interactions between the charges. Hence the derivation of the charge interactions for the microscopic system result in the Coulomb gas formulation of the effective action. We conclude our considerations in chapter 5 with the study of the phase transition. The theory of second order quantum phase transitions is linked to the renormalization group method. Therefore we apply the method to renormalize the partition function. This yields the critical coupling strength for the microscopic system. A similar calculation was shown by P.W. Anderson et al [7] in 1970 for the Coulomb gas formulation of the Kondo problem, which describes the interaction between a magnetic impurity and the electrons in the conduction band.

Basic Concepts

2.1 Dissipative quantum mechanical system

2.1.1 Caldeira-Leggett model

It is not always possible to describe the process of dissipation for a quantum mechanical system from a microscopic point of view. In order to implement dissipation into the quantum mechanical frame work, a model system is employed. In this model the considered system is extended by an environment consisting of a huge number of harmonic oscillators, also called heat bath. The energy loss of the system is transferred to the environment, so that the energy of the global or 'system plus environment'-system is preserved. This model is often named Caldeira-Leggett model, since they used it to study the effects of dissipation on quantum mechanical tunneling processes. If the number of harmonic oscillators is assumed to be huge or infinitely large, the individual coupling to the coordinate of the α -th harmonic oscillator is certainly weak. Then the coupling between the system's coordinate and the α -th harmonic oscillator coordinate is linear. This will be of advantage later on, because linear coupling allows to set up an effective theory where the environment is eliminated. In this case the degrees of freedom of the environment outnumber the degrees of freedom of the system by far, so that energy transfer from the environment back to the system can be completely neglected. The Hamiltonian for the global or total system reads

$$\begin{aligned}
 H &= H_S + H_E + H_I \\
 &= \frac{p^2}{2M} + V(q) + \sum_{\alpha} \left(\frac{p_{\alpha}^2}{2m_{\alpha}} + \frac{1}{2} m_{\alpha} \omega_{\alpha}^2 x_{\alpha}^2 \right) - \sum_{\alpha} x_{\alpha} c_{\alpha} q + \sum_{\alpha} \frac{c_{\alpha}^2 q^2}{2m_{\alpha} \omega_{\alpha}^2}. \quad (2.1)
 \end{aligned}$$

The Hamiltonian is composed of the system part, the environment part and the interaction part. As a system we consider a particle of mass M with momentum p and coordinate q in a potential $V(q)$. The environment is represented by the harmonic oscillators with coordinates x_{α} . The system's coordinate and the individual harmonic oscillator coordinate are linear coupled by the coupling constant c_{α} . The last summand is added due to potential renormalization because of the coupling. The properties of the environmental coupling are described by the spectral

function

$$J(\omega) = \frac{\pi}{2} \sum_{\alpha} \left(\frac{c_{\alpha}^2}{m_{\alpha} \omega_{\alpha}} \right) \delta(\omega - \omega_{\alpha}). \quad (2.2)$$

Dependent on the functional form of the spectral function one distinguishes between three kinds of dissipation. The most interesting case is Ohmic dissipation for which the spectral function is given as

$$J(\omega) = \eta \omega, \quad (2.3)$$

where η is the dissipation coefficient and the frequency ω is supposed to be smaller than some high frequency cutoff ω_c . The Ohmic dissipation is linked to classical mechanics, since the corresponding classical equation of motion has a friction term linear in the dissipation coefficient. The two other cases are defined as

$$J(\omega) \propto \omega^s = \begin{cases} \text{superohmic,} & \text{if } s > 1 \\ \text{subohmic,} & \text{if } 0 < s < 1 \end{cases}. \quad (2.4)$$

For further reading see [3, 4, 8].

2.1.2 Dissipative two state system

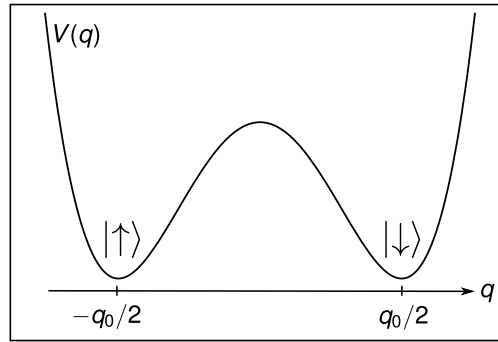


Figure 2.1 The dissipative TSS in the pseudo-spin formulation (adopted from [8]).

If the extent of the potential is restricted to two wells, we are dealing with a double well. Considering the system at a very low temperature the thermal energy is much smaller than the energy gap between the ground state and the excited state of one well. In this case the particle is tied to the ground states of the wells and the only way to get from one well to the other is provided by quantum mechanical tunneling through the potential barrier. Since there are only two possible states available it is named a two state system (TSS). The TSS can be described as a pseudo spin system using the Pauli matrices

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \text{and} \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \quad (2.5)$$

The two possible spin orientations $|\uparrow\rangle$ and $|\downarrow\rangle$ are eigenstates of the Pauli matrix σ_z , which in the double well system are identified with the particle being localized in the right or in the left

well, as shown in Figure 2.1

$$|\uparrow\rangle = |\text{left}\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |\downarrow\rangle = |\text{right}\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \quad (2.6)$$

Applying the σ_z -matrix on its eigenstates yields the eigenvalues $+1$ and -1 , respectively

$$\sigma_z |\text{left}\rangle = +1 |\text{left}\rangle, \quad \sigma_z |\text{right}\rangle = -1 |\text{right}\rangle. \quad (2.7)$$

If we consider a system with minima separation q_0 with the minima to be symmetric relative to the origin at $q = \mp \frac{q_0}{2}$, we can choose a position operator

$$q = -\frac{1}{2} q_0 \sigma_z. \quad (2.8)$$

Acting on the eigenstates, the eigenvalues coincide with the positions of the particle

$$-\frac{1}{2} q_0 \sigma_z |\text{left}\rangle = -\frac{q_0}{2} |\text{left}\rangle, \quad -\frac{1}{2} q_0 \sigma_z |\text{right}\rangle = +\frac{q_0}{2} |\text{right}\rangle. \quad (2.9)$$

In the spin formulation the tunneling between the wells is identified with the umklapp process of the spin. This process is provided by the σ_x matrix of eq. (2.5) acting on the eigenstates of eq. (2.6)

$$\sigma_x |\text{left}\rangle = |\text{right}\rangle, \quad \sigma_x |\text{right}\rangle = |\text{left}\rangle. \quad (2.10)$$

These considerations lead to the Hamiltonian of the global system in the pseudo spin formulation

$$\begin{aligned} H^{\text{SB}} &= H_{\text{TSS}} + H_E + H_I \\ &= -\frac{1}{2} \hbar \Delta \sigma_x + \sum_{\alpha} \left(\frac{p_{\alpha}^2}{2m_{\alpha}} + \frac{1}{2} m_{\alpha} \omega_{\alpha}^2 x_{\alpha}^2 \right) - \frac{1}{2} \sum_{\alpha} q_0 \sigma_z c_{\alpha} x_{\alpha}. \end{aligned} \quad (2.11)$$

The first term describes the tunneling process of the TSS where Δ is the tunneling matrix element with dimension frequency. The second part describes the harmonic environment. The last term describes the linear coupling between the bath of harmonic oscillators and the particle, which is sensitive to the position of the particle. In quantum mechanics the bath of harmonic oscillators can be described as free bosons and since the dynamics of the particle in the well are described as a spin system, the Hamiltonian in eq. (2.11) is named spin boson (SB) Hamiltonian. The strenght of the coupling between the system and the environment is expressed by the dimensionless parameter

$$\alpha = \frac{q_0^2 \eta}{2\pi \hbar}, \quad (2.12)$$

where η is the dissipation coefficient and q_0 the separation between the wells, as shown in Figure 2.2. As mentioned in chapter 1 the coupling strenght is the critical parameter defining the dissipative quantum phase transition. The dissipative TSS exhibits a quantum phase transition at the critical value [4]

$$\alpha_c^{\text{SB}} = 1. \quad (2.13)$$

For coupling strenghts $\alpha < 1$ the particle is nearly unaffected by the environment. It tunnels forth and back between the minima of the double well and thus shows diffusive behavior. In the case of strong coupling with $\alpha > 1$ the influence of the environment leads to the localization of the particle in either one of the wells. A detailed discussion can be found in [3, 4, 8].

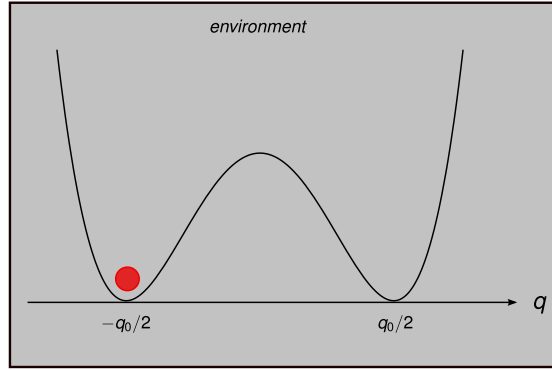


Figure 2.2 The particle in the double well couples to the non-located environment.

SB-Hamiltonian expressed in terms of annihilation and creation operators

For reasons that will become clear later on, it is convenient to replace the position and momentum operators x_α and p_α of the spin-boson-Hamiltonian

$$H_{E,I}^{\text{SB}} = \frac{1}{2} \sum_{\alpha} \left(\frac{p_{\alpha}^2}{m_{\alpha}} + m_{\alpha} \omega_{\alpha}^2 x_{\alpha}^2 \right) - \frac{1}{2} \sum_{\alpha} q_0 \sigma_z c_{\alpha} x_{\alpha}, \quad (2.14)$$

by annihilation and creation operators. We choose the following relations

$$\begin{aligned} x_{\alpha} &= \sqrt{\frac{\hbar}{2m_{\alpha}\omega_{\alpha}}} (b_{\alpha} + b_{\alpha}^{\dagger}) \\ p_{\alpha} &= i\sqrt{\frac{m_{\alpha}\omega_{\alpha}\hbar}{2}} (b_{\alpha}^{\dagger} - b_{\alpha}), \end{aligned} \quad (2.15)$$

where b_{α} and b_{α}^{\dagger} are the bosonic creation and annihilation operators of the α -th harmonic oscillator. Inserting the connection of eq. (2.15) into the environment term yields

$$\begin{aligned} H_E^{\text{SB}} &= \frac{1}{2} \sum_{\alpha} \left(-\frac{\hbar\omega_{\alpha}}{2} (b_{\alpha}^{\dagger} - b_{\alpha})^2 + \frac{\hbar\omega_{\alpha}}{2} (b_{\alpha} + b_{\alpha}^{\dagger})^2 \right) \\ &= \frac{1}{2} \sum_{\alpha} (\hbar\omega_{\alpha} (b_{\alpha}^{\dagger} b_{\alpha} + b_{\alpha} b_{\alpha}^{\dagger})). \end{aligned} \quad (2.16)$$

The expression can be simplified by applying the bosonic commutation relation

$$\begin{aligned} [b_{\alpha}, b_{\alpha}^{\dagger}] &= b_{\alpha} b_{\alpha}^{\dagger} - b_{\alpha}^{\dagger} b_{\alpha} = 1 \\ \Rightarrow b_{\alpha} b_{\alpha}^{\dagger} &= 1 + b_{\alpha}^{\dagger} b_{\alpha}. \end{aligned} \quad (2.17)$$

Inserting the above relation into eq. (2.16) yields

$$\begin{aligned} H_E^{\text{SB}} &= \sum_{\alpha} \left(\frac{1}{2} \hbar\omega_{\alpha} + \hbar\omega_{\alpha} b_{\alpha}^{\dagger} b_{\alpha} \right) \\ &= \sum_{\alpha} E_{0\alpha} + \sum_{\alpha} \hbar\omega_{\alpha} b_{\alpha}^{\dagger} b_{\alpha}. \end{aligned} \quad (2.18)$$

We arrived at the Hamiltonian of the bath consisting of α quantum mechanical oscillators with dispersion relations $\epsilon_\alpha = \hbar\omega_\alpha$ and ground state energies $E_{0\alpha}$. Inserting eq. (2.15) into the interaction term of eq. (2.14) gives

$$\begin{aligned} H_I^{SB} &= -\frac{1}{2} \sum_{\alpha} q_0 \sigma_z c_{\alpha} X_{\alpha} \\ &= -\frac{1}{2} \sum_{\alpha} q_0 \sigma_z c_{\alpha} \sqrt{\frac{\hbar}{2m_{\alpha}\omega_{\alpha}}} (b_{\alpha} + b_{\alpha}^{\dagger}) \\ &= -\frac{1}{2} \sum_{\alpha} q_0 \sigma_z \lambda_{\alpha} (b_{\alpha} + b_{\alpha}^{\dagger}), \end{aligned} \quad (2.19)$$

where we replaced the coupling constant by

$$c_{\alpha} \sqrt{\frac{\hbar}{2m_{\alpha}\omega_{\alpha}}} = \lambda_{\alpha} \Rightarrow c_{\alpha} = \lambda_{\alpha} \sqrt{\frac{2m_{\alpha}\omega_{\alpha}}{\hbar}}. \quad (2.20)$$

The SB Hamiltonian expressed with creation and annihilation operators reads

$$H^{SB} = -\frac{1}{2} \hbar \Delta \sigma_x + \sum_{\alpha} E_{0\alpha} + \sum_{\alpha} \hbar \omega_{\alpha} b_{\alpha}^{\dagger} b_{\alpha} - \frac{1}{2} \sum_{\alpha} q_0 \sigma_z \lambda_{\alpha} (b_{\alpha} + b_{\alpha}^{\dagger}). \quad (2.21)$$

2.2 Construction of the path integral

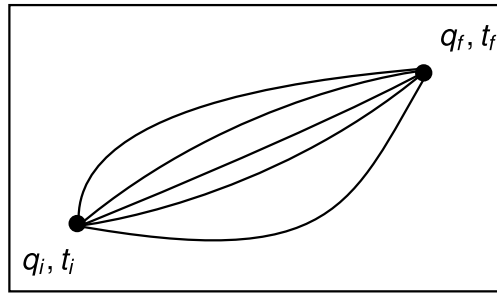


Figure 2.3 The quantum mechanical amplitude for the propagation between the initial point q_i and the final point q_f expressed in the path integral formulation as a sum over the classical path and other possible paths, representing the quantum fluctuations (adopted from [9]).

We follow the calculation presented in [10]. The goal of this section is to find a description for the quantum mechanical amplitude in the classical concept of action. The quantum amplitude for the propagation of a system described by the Hamiltonian H from the initial point q_i at time t_i to the final point q_f at time t_f is given by the matrix element of the time evolution operator

$$\langle q_f, t_f | e^{-i\hat{H}(t_f - t_i)/\hbar} | q_i, t_i \rangle. \quad (2.22)$$

It is convenient not to consider the evolution of the system for the entire time $t = t_f - t_i$, but to monitor the evolution of the system in time slices. This means we are going to insert N time steps Δt with

$$N\Delta t = t = t_f - t_i, \quad (2.23)$$

where N is a large number and hence the time steps are small. This approach allows us to rewrite the amplitude as follows

$$\begin{aligned} \langle q_f | e^{-i\hat{H}(t_f-t_i)/\hbar} | q_i \rangle &= \int dq_{N-1} \dots \int dq_1 \prod_{n=0}^{N-1} \langle q_{n+1} | e^{-i\hat{H}\Delta t/\hbar} | q_n \rangle \\ &= \int dq_{N-1} \dots \int dq_1 \underbrace{\langle q_N |}_{\langle q_f |} e^{-i\hat{H}\Delta t/\hbar} | q_{N-1} \rangle \langle q_{N-1} | e^{-i\hat{H}\Delta t/\hbar} | q_{N-2} \rangle \times \\ &\quad \times \dots \times \langle q_2 | e^{-i\hat{H}\Delta t/\hbar} | q_1 \rangle \langle q_1 | e^{-i\hat{H}\Delta t/\hbar} | \underbrace{q_0}_{| q_i \rangle} \rangle. \end{aligned} \quad (2.24)$$

As the Hamiltonian \hat{H} also depends on the momentum p of the particle we are inserting the identity in momentum space

$$\mathbb{1} = \int dp_n |p_n\rangle \langle p_n|, \quad n = 0, \dots, N-1, \quad (2.25)$$

where the index n indicates the individual time step. The amplitude in eq. (2.24) then becomes

$$\begin{aligned} \langle q_f | e^{-i\hat{H}(t_f-t_i)/\hbar} | q_i \rangle &= \int dq_{N-1} \dots \int dq_1 \int dp_{N-1} \dots \int dp_0 \langle q_N | p_{N-1} \rangle \langle p_{N-1} | e^{-i\hat{H}\Delta t/\hbar} | q_{N-1} \rangle \times \\ &\quad \times \dots \times \langle q_{N-1} | p_{N-2} \rangle \langle p_{N-2} | e^{-i\hat{H}\Delta t/\hbar} | q_{N-2} \rangle \langle q_1 | p_0 \rangle \langle p_0 | e^{-i\hat{H}\Delta t/\hbar} | q_0 \rangle. \end{aligned} \quad (2.26)$$

The propagation of the particle in the classical phase space is split in N time slices. The Baker-Campbell-Hausdorff formula allows us to split the time evolution operator into the kinetic energy and the potential energy operator, if $(\Delta t)^2$ is negligible small

$$\langle p_n | e^{-i\hat{H}\Delta t/\hbar} | q_n \rangle \stackrel{\mathcal{O}(\Delta t)}{=} \langle p_n | e^{-i\hat{T}(\hat{p})\Delta t/\hbar} e^{-i\hat{V}(\hat{q})\Delta t/\hbar} | q_n \rangle. \quad (2.27)$$

Obviously the derivation is only valid for Hamiltonians of the form $\hat{H} = \hat{T} + \hat{V}$. As the kinetic energy operator is a function of the momentum operator and the potential energy operator a function of the position operator the expression in eq. (2.27) allows the operators to act on their momentum and position eigenstates respectively. In this case the operators can be replaced by their eigenvalues

$$e^{\hat{V}(\hat{q})} | q \rangle = \sum_{k=0}^{\infty} \frac{(\hat{V}(\hat{q}))^k}{k!} | q \rangle = \sum_{k=0}^{\infty} \frac{(V(q))^k}{k!} | q \rangle = e^{V(q)} | q \rangle. \quad (2.28)$$

The same holds for the kinetic energy operator, so that eq. (2.27) yields

$$\langle p_n | e^{-i\hat{T}(\hat{p})\Delta t/\hbar} e^{-i\hat{V}(\hat{q})\Delta t/\hbar} | q_n \rangle = e^{-i(T(p_n)+V(q_n))\Delta t/\hbar} \langle p_n | q_n \rangle. \quad (2.29)$$

We make use of the fact, that the position and the momentum representation are connected via Fourier transformation

$$\langle p_n | q_n \rangle = \langle q_n | p_n \rangle^* = e^{-ip_n q_n/\hbar}, \quad (2.30)$$

thus the matrix element in eq. (2.29) becomes

$$\langle p_n | e^{-i\hat{T}(\hat{p})\Delta t/\hbar} e^{-i\hat{V}(\hat{q})\Delta t/\hbar} | q_n \rangle = e^{-i(T(p_n)+V(q_n))/\hbar} e^{-ip_n q_n/\hbar}. \quad (2.31)$$

These considerations can be applied to the amplitude in eq. (2.26)

$$\begin{aligned}
\langle q_f | e^{-i\hat{H}(t_f-t_i)/\hbar} | q_i \rangle &= \int dq_{N-1} \dots \int dq_1 \int dp_{N-1} \dots \int dp_0 e^{\frac{i}{\hbar} q_N p_{N-1}} e^{-\frac{i}{\hbar} (T(p_{N-1})+V(q_{N-1}))} \times \\
&\quad \times e^{-\frac{i}{\hbar} p_{N-1} q_{N-1}} \dots e^{\frac{i}{\hbar} q_1 p_0} e^{-\frac{i}{\hbar} (T(p_0)+V(q_0))} e^{-\frac{i}{\hbar} p_0 q_0} \\
&= \int dq_{N-1} \dots \int dq_1 \int dp_{N-1} \dots \int dp_0 e^{-\frac{i}{\hbar} \sum_{n=0}^{N-1} (T(p_n)+V(q_n)) \Delta t} \times \\
&\quad \times e^{-\frac{i}{\hbar} \sum_{n=0}^{N-1} (-p_n(q_{n+1}-q_n))} \\
&= \int dq_{N-1} \dots \int dq_1 \int dp_{N-1} \dots \int dp_0 e^{-\frac{i}{\hbar} \sum_{n=0}^{N-1} [T(p_n)+V(q_n)-p_n(\frac{q_{n+1}-q_n}{\Delta t})]} \Delta t
\end{aligned} \tag{2.32}$$

To gain the path integral formulation of the quantum mechanical amplitude we consider eq. (2.32) in the limit $N \rightarrow \infty$ with $t = N\Delta t$ fixed

$$\langle q_f | e^{-i\hat{H}t/\hbar} | q_i \rangle = \int \mathcal{D}[q] \int \mathcal{D}[p] e^{\frac{i}{\hbar} \int_0^T dt (p\dot{q} - H(p,q))}, \tag{2.33}$$

where we have chosen the initial time to be zero and the final time to be T . This is the Hamilton formulation of the path integral, where the integrations in the phase space are expressed as a functional or path integral in the coordinate q and the momentum p . To connect the quantum mechanical amplitude to the classical action, we have to switch to the Lagrange formalism, which only depends on the coordinate q . Since the kinetic energy is quadratic in the momentum variable, the path integration over the variable q can be carried out by applying the functional Gaussian integration. We then get

$$\langle q_f | e^{-i\hat{H}t/\hbar} | q_i \rangle = \int_{q_i}^{q_f} \mathcal{D}[q] e^{i/\hbar \int_0^T dt L(q,\dot{q})} = \int_{q_i}^{q_f} \mathcal{D}[q] e^{i/\hbar S(q)}, \tag{2.34}$$

where L is the Lagrange function and S the action of the system. One can interpret, that the propagation between two points in quantum mechanics is gained by considering quantum fluctuations around the classical path. All reasonably smooth paths connecting the initial and the final point are added up, each weighted by its classical action shown in Figure 2.3. The biggest contribution is provided by the classical path, because the phases of the quantum fluctuations are nearly canceling each other. For further reading see [11].

2.3 Statistical mechanics

A canonical ensemble describes a system in contact with a much larger heat bath, that fixes the temperature T . Only energy transfer between the system and the bath is allowed. If the system is not fully prepared, the quantum mechanical state of the system is not determined. This is called a mixed state. In order to describe this uncertainty one considers possible pure states $|\Psi_r\rangle$ of the system that have energies E_r and occur with the probability

$$P_r = \frac{1}{Z} e^{-\frac{E_r}{k_B T}} = \frac{1}{Z} e^{-\beta E_r}. \tag{2.35}$$

The partition function Z describes the sum of all states the system could possibly capture. This means they have to comply with the conditions that are dictated by the bath. I.e. the energy

values E_r of the possible states have to be small, since the system's energy is much smaller than the energy of the bath. Every state $|\Psi_r\rangle$ is weighted by the Boltzmann factor $e^{-\beta E_r}$ where k_B is the Boltzmann constant. The probability to find the system in any state must equal one

$$\sum_r P_r = \sum_r \frac{1}{Z} e^{-\beta E_r} = 1. \quad (2.36)$$

The partition function of the canonical ensemble can therefore be deduced from the normalization condition

$$Z = \sum_r e^{-\beta E_r} = \text{tr} \left(e^{-\beta H} \right) = \sum_r \langle \Psi_r | e^{-\beta H} | \Psi_r \rangle. \quad (2.37)$$

The partition function is the sum over all diagonal matrix elements of the canonical operator $e^{-\beta H}$ with eigenenergies E_r and eigenstates $|\Psi_r\rangle$. The density operator of the mixed state is given by

$$\rho = \sum_r P_r |\Psi_r\rangle \langle \Psi_r| \stackrel{(2.35)}{=} \frac{1}{Z} \sum_r |\Psi_r\rangle e^{-\beta E_r} \langle \Psi_r|. \quad (2.38)$$

If the system is fully prepared due to measurements, there is no uncertainty and the probability to find the system in the state $|\Psi\rangle$ equals one, hence the density operator becomes the projection operator. A more detailed explanation can be found in [12].

2.4 Path integral and statistical mechanics

The canonical partition function is linked to the quantum mechanical amplitude by the so called Wick rotation, which leads to a path integral description of statistical mechanics in imaginary time. The partition function is obtained from the canonical density operator by a trace operation, that means a summation over all diagonal matrix elements of the canonical density operator

$$\begin{aligned} Z &= \text{tr} \left(e^{-\beta H} \right) \\ &= \int dq \langle q | e^{-\beta H} | q \rangle, \quad \text{with} \quad \beta = \frac{1}{k_B T}. \end{aligned} \quad (2.39)$$

The partition function describes the number of all possible equilibrium configurations of the considered system. To see the connection to the path integral formalism we consider the quantum amplitude in imaginary time, which can be derived by the Wick rotation

$$\tau = it. \quad (2.40)$$

We then have for the amplitude

$$\langle q_f | e^{-iHt/\hbar} | q_i \rangle \xrightarrow{\tau=it} \langle q_f | e^{-\tau H/\hbar} | q_i \rangle. \quad (2.41)$$

The arguments given in section 2.2 for the derivation of the path integral in real time, still hold for the description in imaginary time. Thus the form of the path does not change, but we have to take into account that the Lagrange function in the exponent has to be Wick transformed too. We therefore have to transform the differential operator from real to imaginary time

$$t = i\tau \Rightarrow \partial_t = -i\partial_\tau. \quad (2.42)$$

The action reads

$$S = \int dt L(q, \dot{q}) = \int dt \left(\frac{M}{2} (\partial_t q)^2 - V(q) \right). \quad (2.43)$$

With the relation of eq. (2.42), we then obtain

$$S = -i \int d\tau \left(\frac{M}{2} i^2 (\partial_\tau q)^2 + V(q) \right). \quad (2.44)$$

Since the kinetic energy is supposed to be a positive quantity, the sign of the potential changes

$$S = -i (i^2) \int d\tau \left(\frac{M}{2} (\partial_\tau q)^2 + V(q) \right) \quad (2.45)$$

$$\begin{aligned} &= i \int d\tau \left(\frac{M}{2} (\partial_\tau q)^2 + V(q) \right) \\ &= i \int d\tau L^E(q, \partial_\tau q) = iS^E, \end{aligned} \quad (2.46)$$

where the Lagrangian and the action are called Euclidean, indicated by the superscript E. We are now able to write down a path for the amplitude in imaginary time

$$\langle q_f | e^{-\frac{H\tau}{\hbar}} | q_i \rangle = \int_{q_i}^{q_f} \mathcal{D}[q] e^{-\frac{1}{\hbar} \int d\tau L^E(q, \partial_\tau q)}. \quad (2.47)$$

In order to identify this formulation with the partition function, we have to consider the case where the initial point and the final point of the path are the same

$$q_i(\tau_i) = q_f(\tau_f). \quad (2.48)$$

This can be archived by making the imaginary time periodical, then the path is closed in time. Our choice for the imaginary time connects the Planck constant with the temperature

$$\tau = \hbar\beta. \quad (2.49)$$

Now the connection with statistical mechanics becomes obvious,

$$\langle q_f | e^{-\frac{\tau H}{\hbar}} | q_i \rangle \stackrel{\tau = \hbar\beta}{=} \langle q | e^{-\beta H} | q \rangle. \quad (2.50)$$

Now we can rewrite the partition function in terms of the path integral

$$Z = \int_{q_i=q_f}^{q_f} \mathcal{D}[q] e^{-\frac{1}{\hbar} \int_0^{\hbar\beta} d\tau L^E(q, \partial_\tau q)} \quad (2.51)$$

In the case of the Caldeira-Leggett model the Euclidean Lagrange function also depends on the coordinates \mathbf{x} of the environment

$$\begin{aligned} L^E(q, \partial_\tau q, \mathbf{x}) &= L_S^E(q, \partial_\tau q) + L_E^E(\mathbf{x}) + L_I^E(q, \mathbf{x}) \\ &= \frac{M}{2} \dot{q}^2 + V(q) + \frac{1}{2} \sum_{\alpha} m_{\alpha} (\dot{x}_{\alpha}^2 + \omega_{\alpha}^2 x_{\alpha}^2) - \sum_{\alpha} c_{\alpha} x_{\alpha} q + \sum_{\alpha} \frac{1}{2} \frac{c_{\alpha}^2 q^2}{m_{\alpha} \omega_{\alpha}^2}, \end{aligned} \quad (2.52)$$

The partition function for the total system is then given by

$$Z_{\text{tot}} = \int_{q_i=q_f}^{q_f} \mathcal{D}[q] \int_{x_i=x_f}^{x_f} \mathcal{D}[x] e^{-\frac{1}{\hbar} \int_0^T d\tau L^E(q, \partial_\tau q, x)}. \quad (2.53)$$

A more detailed derivation can be found in [9, 10].

2.5 Bose Einstein condensation (BEC)

At high temperatures the Bose gas satisfies the Maxwell Boltzmann statistic of a classical gas, so the quantum nature of the particles is not apparent for high temperatures. If we are dealing with a cold gas at very low temperatures, quantum mechanical effects will become important. Thus we have to distinguish between fermions and bosons. In order to see the effect of cooling in the Bose gas we are describing it in the grand canonical ensemble, which is an extension of the canonical ensemble since the system can exchange energy and particles with the bath. The average energy of the system is given as the sum of the eigenenergies of the quantum mechanical states multiplied by the average occupation number of that state

$$\bar{E} = \sum_k \bar{n}_k E_k. \quad (2.54)$$

The average number of particles in the gas equals the sum over all average occupation numbers

$$\bar{N} = \sum_k \bar{n}_k. \quad (2.55)$$

The average occupation number for bosons is given by the Bose Einstein statistic

$$\bar{n}_k = \frac{1}{e^{\beta(E_k - \mu)} - 1} \quad \text{with} \quad \mu \leq E_k, \quad (2.56)$$

where μ is the chemical potential that can be physically interpreted as the amount of energy that is necessary to add a boson to the system. As multiple bosons can occupy the same quantum mechanical state, the average occupation number can be larger than one. For a given temperature the average occupation of quantum states with small energies is bigger than for quantum states with larger energies. On the contrary, the average occupation number for fermions given by the Fermi-Dirac statistic lies between zero and one due to the Pauli principle. We are now interested how the properties of the gas change if the temperature tends to zero. We therefore look at the behavior of the average occupation number

$$\lim_{T \rightarrow 0} \sum_k \bar{n}_k = 0 \quad (2.57)$$

This result is a serious problem, since the total number of particles would be zero, which is no physical acceptable conclusion. In order to solve this contradiction one can assume that at $T = 0$ the ground state of the system is macroscopically occupied. This means that all the bosons in the gas enter the ground state with ground state energy E_0 , that equals the chemical potential and is chosen to be zero. The gas of free bosons enters for a critical temperature T_c a new phase that is called a Bose Einstein condensate (BEC). For temperatures under the

critical temperature and above $T = 0$ there are still bosons out of the condensate, but their number becomes zero for $T = 0$. This situation is described by the momentum distribution of the occupation number with $\mu = 0$

$$n(\mathbf{p}) = N_0 \delta(\mathbf{p}) + \frac{V}{(2\pi\hbar)^3} \frac{1}{\exp(\beta p^2/2m) - 1}, \quad (2.58)$$

where N_0 is the number of particles in the condensate. We can approximate

$$\frac{1}{\exp(\beta p^2/2m) - 1} \approx \frac{2mk_B T}{p^2}. \quad (2.59)$$

Hence we obtain for a three-dimensional bose gas at zero temperature

$$\int d^3\mathbf{p} n(\mathbf{p}) = N_0. \quad (2.60)$$

In $2D$ and $1D$ the term in eq. (2.59) leads to a divergence in the above integral. This is why a BEC can only occur in $3D$. The phase transition of an ideal bose gas to a BEC was first predicted by A. Einstein and S. Bose in 1925. The experimental realization was achieved much later in 1995 with isotopes of Rubidium, Sodium, as well as Lithium. The creation of a BEC is technically very demanding, since the gas has to be cooled down to very low temperatures and has to be confined in a potential trap. For further reading see [12, 13].

2.6 Bogoliubov theory

We follow the calculation presented in [13]. The physics of an ideal Bose gas at $T = 0$ has been discussed previously. One must expect a deviation from these properties, when the ideal description is dropped and interactions are taken into account. We are going to see how a weakly interacting Bose condensate can be treated mathematically to derive the dispersion relation. A technique was provided by Nicolay Bogoliubov in 1947, the so called Bogoliubov theory.

Since the gas is supposed to be weakly interacting it has to be dilute. In this case the average distance between the particles is bigger than the range of the interaction forces. So it is sufficient to consider only two particle interactions. At the temperature $T = 0$ we are dealing with very low energies and hence small momenta. It is then justified to describe the scattering process in lowest order, namely s-wave scattering with scattering length a . In this case the process is not dependent on angles and the angular momentum is zero. The Hamiltonian for a Bose gas considering interactions between two particles with momenta p_1 and p_2 is given by

$$H = \sum_p \frac{p^2}{2m} a_p^\dagger a_p + \frac{V_0}{2V} \sum_{p_1, p_2, q} a_{p_1+q}^\dagger a_{p_2-q}^\dagger a_{p_1} a_{p_2}, \quad (2.61)$$

where V is the occupied volume, m the mass of the boson and a_p and a_p^\dagger are the bosonic annihilation and creation operators. V_0 is the Fourier transformed effective potential for zero momentum. The first term describes the kinetic energy and the second term describes the interaction process where the particles with initial momenta p_1 and p_2 are annihilated and two particles with momenta $p_1 + q$ and $p_2 - q$ are created. The first order approximation of the Hamiltonian would be to neglect all terms with momentum $p \neq 0$ which gives the ground state

energy E_0 . To obtain the dispersion relation one has to take at least terms which are quadratic in the annihilation and creation operators for non zero momenta into account and arrives at

$$H = \frac{V_0}{2V} a_0^\dagger a_0^\dagger a_0 a_0 + \sum_p \frac{p^2}{2m} a_p^\dagger a_p + \frac{V_0}{2V} \sum_{p \neq 0} \left(4a_0^\dagger a_p^\dagger a_0 a_p + a_p^\dagger a_{-p}^\dagger a_0 a_0 + a_0^\dagger a_0^\dagger a_p a_{-p} \right). \quad (2.62)$$

In a gas at temperature $T = 0$ almost all bosons are in the ground state with momentum $p = 0$. In this case it is legitimate to replace the annihilation and creation operators for $p = 0$ by their eigenvalues

$$a_0 = \sqrt{N_0}, \quad a_0^\dagger \stackrel{N_0 \gg 1}{=} \sqrt{N_0}, \quad (2.63)$$

where N_0 is the number of particles in the ground state. In contrast to the ideal bose condensate, even at $T = 0$ not all of the N bosons in the weakly interacting gas enter the ground state. Due to the interactions a small number of particles remains out of the condensate, which is called quantum depletion. Hence the normalization condition for the particles is

$$N = \sum_{p \neq 0} a_p^\dagger a_p + a_0^\dagger a_0. \quad (2.64)$$

Using the relation of eq. (2.64) and the results of perturbation theory connecting the effective potential V_0 , the collision parameter g and the scattering length a , one can rewrite the Hamiltonian and obtains

$$H = g \frac{N^2}{2V} + \frac{p^2}{2m} a_p^\dagger a_p + \sum_p + \frac{1}{2} gn \sum_{p \neq 0} \left(2a_p^\dagger a_p + a_p^\dagger a_{-p}^\dagger + a_p a_{-p} + \frac{mng}{p^2} \right), \quad (2.65)$$

with m being the mass of the bosons. The Bogoliubov transformation replaces the bosonic annihilation and creation operators a_p and a_p^\dagger by the Bogoliubov operators b_p and b_p^\dagger that also obey the bosonic commutation relation

$$\begin{aligned} a_p &= u_p b_p + v_{-p}^* b_{-p}^\dagger, \\ a_p^\dagger &= u_p^* b_p^\dagger + v_{-p} b_{-p}. \end{aligned} \quad (2.66)$$

The coefficients of the transformation

$$u_p = \left(\frac{p^2}{2m} + \frac{gn}{2} + \frac{1}{2} \right)^{\frac{1}{2}}, \quad v_{-p} = - \left(\frac{p^2}{2m} + \frac{gn}{2} - \frac{1}{2} \right)^{\frac{1}{2}}, \quad (2.67)$$

are chosen to cancel the off-diagonal terms in the Hamiltonian. Thus the Bogoliubov transformation is a method of diagonalization. Applying the relations of eq. (2.66) and eq. (2.67) to the Hamiltonian in eq. (2.65) one obtains the diagonal Hamiltonian

$$H = E_0 + \sum_p \epsilon(p) b_p^\dagger b_p, \quad (2.68)$$

where the ground state energy in contrast to the ideal bose gas is non zero due to the interactions. The analogy to the energy spectrum of the quantum harmonic oscillator becomes apparent. In this sense the BEC of weakly interacting bosons can be described as a system with ground state energy E_0 consisting of independent or noninteracting quasi-particles with

energies $\epsilon(p)$ that are annihilated and created by the Bogoliubov operators. One has to keep in mind, that the new description formally describes free bosons, but nonetheless incorporates the interactions between the bosons. This technical simplification of the problem is the advantage of the Bogoliubov theory. The dispersion relation of the system is given by

$$\epsilon(p)^2 = \frac{gnp^2}{m} + \left(\frac{p^2}{2m}\right)^2. \quad (2.69)$$

The excitations of the system are identified as sound waves with the sound velocity

$$v_s = \sqrt{\frac{gn}{m}}, \quad (2.70)$$

with a phonon like dispersion relation.

2.7 Tight binding (TB) model and charge picture

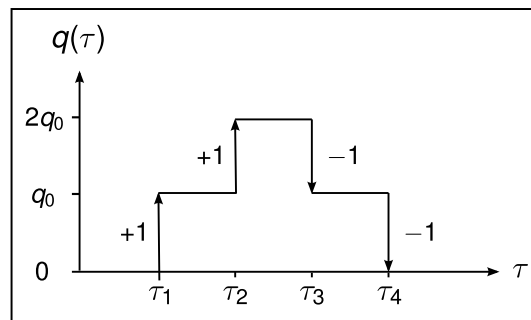


Figure 2.4 TB path with two kinks and antikinks, indicated as arrows (adopted from [8]).

If the energy of a particle in a harmonic potential is too small to overcome the barrier between the wells, it is tied to the minima of the potential. The only way to get from one minimum to the neighboring minimum is by quantum mechanical tunneling, which is called a tight binding (TB) path. If the energy of the particle is larger than the potential energy the particle barely senses the presence of the potential and can move nearly unaffected by it. In analogy this case is called a weak binding (WB) model, where the coordinate of the particle is continuous. On the contrary,

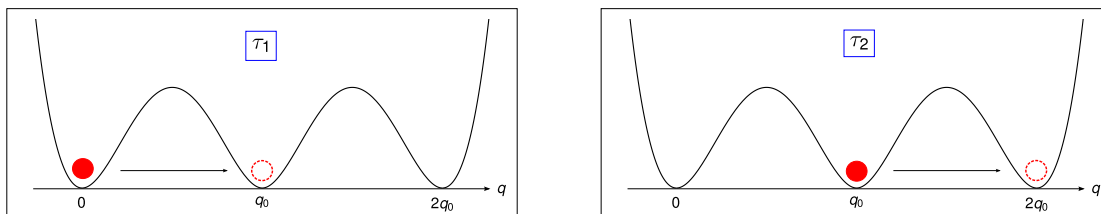


Figure 2.5 The left panel shows the first move of the particle at τ_1 and the right panel the next move at τ_2 .

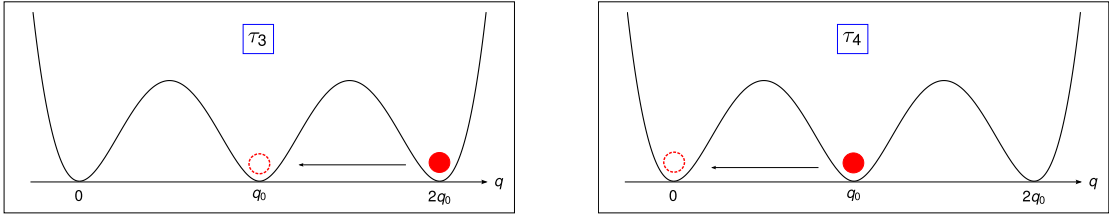


Figure 2.6 The particle moves back at times τ_3 and τ_4 .

the strong influence of the potential in the TB model forces the path $q(\tau)$ of the particle to be discrete

$$q(\tau) = q_0 k(\tau) \quad (2.71)$$

where q_0 is the distance between two minima, also called TB lattice constant and $k(\tau)$ is a dimensionless function that only takes integer values $0, \pm 1, \pm 2, \dots$. So the particle is always localized in the minima of the wells

$$q(\tau) = \left[0, \pm q_0, \pm 2q_0, \pm 3q_0, \dots, \pm \frac{K}{2} q_0 \right], \quad (2.72)$$

where K is the total number of wells. The tunneling process between two minima can be assumed to be instantaneous, so that the TB path can be described by the step function

$$\theta(\tau - \tau_i) = \begin{cases} 1, & \text{if } \tau > \tau_i \\ 0, & \text{if } \tau < \tau_i \end{cases}, \quad (2.73)$$

An arbitrary path can be built by adding up step functions

$$q(\tau) = q_0 \sum_i e_i \theta(\tau - \tau_i), \quad (2.74)$$

where the step size q_0 equals the tunneling length, if the particle tunnels exclusively between two neighboring minima. In this case going forward at τ_i in the potential means adding a step function with positive sign $e_i = +1$. Going backward or to the left at τ_i in analogy means adding a step function with negative sign $e_i = -1$. In Figure 2.5 and Figure 2.6 we show a sequence of tunneling processes and in Figure 2.4 the related TB path. The path in Figure 2.4 is made up of equally long segments, but in general the time period between two kinks/antikinks is not identical, since the particle can stay an arbitrary time in each well. The arrows show the direction of the moves, which are also named

$$\begin{aligned} \text{kink} &\rightarrow \text{move upward,} \\ \text{antikink} &\rightarrow \text{move downward.} \end{aligned} \quad (2.75)$$

The TB path can be formulated equivalently in the charge picture, if the sign of the step function is identified as a positive or negative charge e_i

$$\begin{aligned} \text{kink} &\rightarrow +1, \\ \text{antikink} &\rightarrow -1, \end{aligned} \quad (2.76)$$

τ_1	τ_2	τ_3	...	τ_n
↓	↓	↓		↓
e_1	e_2	e_3	...	e_n

Table 2.1

which is shown for the exemplary path in Figure. For a general path with n kinks and antikinks we can assign the charges $e_i \pm 1$ to the kinks/antikinks at τ_i shown in Table 2.1. In order to formulate the partition function in the charge picture later on, we introduce the neutrality condition

$$\sum_i e_i \stackrel{!}{=} 0, \quad (2.77)$$

which requires the number of positive and negative charges to be equal, i.e. the particle moves as many times forward as backwards and thus always comes back to the initial well. A detailed description can be found in [8].

Mapping between the microscopic and the spin-boson-system

3.1 The microscopic system

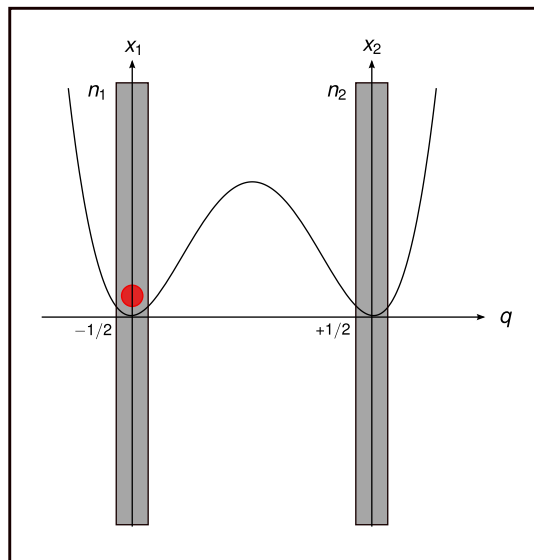


Figure 3.1 The microscopic double well. The two minima are overlaid with bose tubes with densities n_1 and n_2 , respectively.

We are considering one particle in a one dimensional harmonic potential at zero temperature. The minima of the potential are overlaid with one dimensional Bose-Einstein-condensates, also called bose tubes, which represent the dissipative environment. The localization of the tubes in the minima requires a new description of the coupling between the particle and the environment. We are going to describe the system microscopically. Hence the system will be called microscopic system. First, we are going to look at the double well with two bose tubes, which can be

seen in Figure 3.1. In order to determine the physical properties of the system, as described by the spectral function, we are going to map the microscopic Hamiltonian onto the spin-boson Hamiltonian describing the dissipative two state system. After that we will expand the double well as a lattice. In the derivation of the microscopic Hamiltonians we follow the arguments presented in Jaksch et al [14] for cold atoms in an optical lattice.

3.2 Derivation of the microscopic Hamiltonian describing the double well

The two state system

The TSS has been explained in section 2.1.2. In the microscopic formulation the tunneling process is expressed as the annihilation of a particle being localized in one well and the creation of a particle being localized in the other well

$$H_{\text{TSS}}^{\text{mic}} = -J(c_{\uparrow}^{\dagger}c_{\downarrow} + c_{\downarrow}^{\dagger}c_{\uparrow}), \quad (3.1)$$

where J is the hopping matrix element and is of dimension energy. The first term annihilates the particle in the right well and creates a particle in the left well. The second term describes the reverse situation

$$c_{\uparrow}^{\dagger}c_{\downarrow}|\uparrow\rangle = 0, \quad c_{\uparrow}^{\dagger}c_{\downarrow}|\downarrow\rangle = |\uparrow\rangle, \quad c_{\downarrow}^{\dagger}c_{\uparrow}|\uparrow\rangle = |\downarrow\rangle, \quad c_{\downarrow}^{\dagger}c_{\uparrow}|\downarrow\rangle = 0. \quad (3.2)$$

In matrix notation this can be described as follows

$$c_{\uparrow}^{\dagger}c_{\downarrow} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad c_{\downarrow}^{\dagger}c_{\uparrow} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}. \quad (3.3)$$

The sum of the matrices gives the σ_x matrix

$$\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \sigma_x. \quad (3.4)$$

Hence the TSS Hamiltonian can be described in Pauli notation as

$$H_{\text{TSS}}^{\text{mic}} = -J\sigma_x. \quad (3.5)$$

The interaction

The interaction between the particle and the bose tube is state dependent. If the particle is in the left well, it couples to the bose tube 1 with density n_1 . If the particle is in the right well it couples to the bose tube 2 with density n_2 . This can be described by the projection operators

$$P_{\uparrow} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \frac{1}{2}(\sigma_z + \mathbb{1}) \quad \text{and} \quad P_{\downarrow} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = \frac{1}{2}(\mathbb{1} - \sigma_z). \quad (3.6)$$

The projection operator checks whether the particle is in the left or in the right well respectively. The interaction Hamiltonian can be written as

$$H_I^{\text{mic}} = \frac{1}{2}(\sigma_z + \mathbb{1})U_1 + \frac{1}{2}(\mathbb{1} - \sigma_z)U_2. \quad (3.7)$$

U describes the microscopic interaction between the quantum mechanical probability density of the particle in the well and the density of the bose tube

$$\begin{aligned} U_{1,2} &= \int d^3x |\Psi_T(\mathbf{x})|^2 n_{1,2}(0) g_{ab} \\ &= n_{1,2} g_{ab}, \end{aligned} \quad (3.8)$$

where we have applied the normalization condition for the probability density

$$\int d^3x |\Psi_T(\mathbf{x})|^2 = 1. \quad (3.9)$$

g_{ab} is the collision parameter between the particle in the well and a boson in the tube. Since we consider a one dimensional tube the collision parameter is of dimension energy times length and the density is of dimension one over length and hence U is of dimension energy. The bose tubes are placed symmetrically relative to the minima and thus the particle in the minimum couples to the densities $n_{1,2}(x=0)$.

Expanding eq. (3.7) yields

$$H_I^{\text{mic}} = \frac{1}{2} \sigma_z g_{ab} (n_1(0) - n_2(0)) + \frac{1}{2} g_{ab} (n_1(0) + n_2(0)) \quad (3.10)$$

The σ_z - matrix only appears in the first term and hence only the antisymmetric mode of the tubes is sensitive to the position of the particle. The antisymmetric mode equals the difference of the densities

$$\begin{aligned} \text{antisymmetric mode} &\rightarrow n_1(0) - n_2(0) \\ \text{symmetric mode} &\rightarrow n_1(0) + n_2(0). \end{aligned} \quad (3.11)$$

We can conclude that the particle couples exclusively to the antisymmetric mode of the tubes. The analogy of the BEC to the harmonic oscillator provided by the Bogoliubov theory gives rise to a physical picture. The symmetric and antisymmetric mode can be explained as the oscillators of both tubes swinging in phase and out of phase respectively. Since the symmetric mode is not relevant for the coupling we can drop the second term.

The environment

The bose tubes are one dimensional Bose-Einstein condensates. In order to describe the environment microscopically we apply the Bogoliubov theory of weakly interacting bosons under the critical temperature. Since there is no interaction between the tubes the Hamiltonian of the environment is the sum of the Hamiltonians of each tube

$$\begin{aligned} H_E^{\text{mic}} &= H_{E1}^{\text{mic}} + H_{E2}^{\text{mic}} \\ &= E_{01} + \sum_p \epsilon(p) b_{p1}^\dagger b_{p1} + E_{02} + \sum_p \epsilon(p) b_{p2}^\dagger b_{p2}, \end{aligned} \quad (3.12)$$

with ground state energies $E_{0(1,2)}$ and harmonic excitations $\epsilon(p)$. The annihilation and creation operators are the bosonic Bogoliubov operators. The operators are distinguishable by the indices 1 and 2 indicating which bose tube they describe. Since the bose tubes are assumed to be identical in their physical properties, the ground state energies and the dispersion relations

are the same. The considerations of this section lead to the Hamiltonian of the microscopic double well

$$\begin{aligned} H_{\text{double}}^{\text{mic}} &= H_{\text{TSS}}^{\text{mic}} + H_{\text{E}}^{\text{mic}} + H_{\text{I}}^{\text{mic}} \\ &= -J\sigma_x + E_{01} + E_{02} + \sum_p \epsilon(p) b_{p1}^\dagger b_{p1} + \sum_p \epsilon(p) b_{p2}^\dagger b_{p2} + \frac{1}{2} g_{\text{ab}} \sigma_z (n_1(0) - n_2(0)) \end{aligned} \quad (3.13)$$

The spin-boson-Hamiltonian of the two state system in a dissipative environment represented by α harmonic oscillators was introduced in section 2.1.2 and reads

$$\begin{aligned} H^{\text{SB}} &= H_{\text{TSS}}^{\text{SB}} + H_{\text{E}}^{\text{SB}} + H_{\text{I}}^{\text{SB}} \\ &= -\frac{1}{2} \hbar \Delta \sigma_x + \sum_{\alpha} E_{0\alpha} + \sum_{\alpha} \hbar \omega_{\alpha} b_{\alpha}^\dagger b_{\alpha} + -\frac{1}{2} \sum_{\alpha} q_{0\sigma_z} \lambda_{\alpha} (b_{\alpha} + b_{\alpha}^\dagger). \end{aligned} \quad (3.14)$$

The advantage of expressing the SB-Hamiltonian in terms of annihilation and creation operators, as shown in section 2.1.2, becomes now apparent. The mapping between the Hamiltonians requires that they are expressed in the same mathematical form.

3.3 Mapping between the Hamiltonians describing the double well

3.3.1 Mapping between the TSS-Hamiltonians

In the case of the SB-system and the microscopic system, respectively, the motion of the particle in the double well is described as follows

$$H_{\text{TSS}}^{\text{mic}} = -J\sigma_x, \quad H_{\text{TSS}}^{\text{SB}} = -\frac{1}{2} \hbar \Delta \sigma_x. \quad (3.15)$$

The comparison of the above Hamiltonians yields the relation between the hopping matrix element J and the tunneling matrix element Δ

$$J = \frac{1}{2} \hbar \Delta, \quad (3.16)$$

where J is of dimension energy and Δ is of dimension frequency.

3.3.2 Environment mapping

The microscopic and the spin-boson Hamiltonians describing the environment of the two systems

$$H_{\text{E}}^{\text{SB}} = \sum_{\alpha} E_{0\alpha} + \sum_{\alpha} \hbar \omega_{\alpha} b_{\alpha}^\dagger b_{\alpha}, \quad (3.17)$$

$$H_{\text{E}}^{\text{mic}} = E_{01} + \sum_p \epsilon(p) b_{p1}^\dagger b_{p1} + E_{02} + \sum_p \epsilon(p) b_{p2}^\dagger b_{p2}, \quad (3.18)$$

can now be compared. In the spin-boson system the environment consists of α harmonic oscillators and in the microscopic system the environment consists of p harmonic oscillators. In

this spirit the indices have the same meaning and can be interchanged. Hence we can write $\omega_\alpha = \omega(p)$. The mapping thus yields

$$\epsilon(p) = \hbar\omega(p), \quad (3.19)$$

where $\epsilon(p)$ is the Bogoliubov dispersion relation and ω the frequency of the p -th harmonic oscillator. The ground state energies of the systems can be mapped, too

$$E_{01} + E_{02} = \sum_{\alpha} E_{0\alpha}. \quad (3.20)$$

Since they are only an energy offset, they are not relevant for the physical description and can be dropped.

3.3.3 Interaction mapping

The mapping between the interaction Hamiltonians provides the most important physical information about the microscopic system. We can identify the coupling constant for the microscopic system. Together with the Bogoliubov coefficients and the dispersion relation describing the environment we can derive the spectral function eq. (2.2). The form of the function determines whether the dissipation is ohmic or not. The mapping between the interaction terms of eq. (3.13) and eq. (3.14), respectively, can not yet be done.

Microscopic interaction Hamiltonian expressed in terms of annihilation and creation operators

The mapping of the interaction term

$$H_I^{\text{mic}} = \frac{1}{2} \sigma_z g_{ab} (n_1(0) - n_2(0)), \quad (3.21)$$

requires a description of the real space densities $n_{1,2}(0)$ in terms of bosonic creation and annihilation operators in momentum space. This can be achieved by applying the Fourier transformation followed by a Bogoliubov transformation. The densities n_i in real space and n_p in momentum space are related via Fourier transformation

$$n_i = \frac{1}{V} \sum_p n_p e^{ipx_i} = \Psi_i^\dagger \Psi_i, \quad (3.22)$$

where x_i is the coordinate, p the momentum and V the volume of the condensate with dimension one over length. The Ψ_i^\dagger and Ψ_i are the creation and annihilation operators in position representation. Since we are dealing with a one dimensional bose tube the density and the volume have dimension one over length. The inverse transformation is continuous

$$\begin{aligned} n_p &= \int dx_i n_i e^{-ipx_i} \\ &= \int dx_i \Psi_i^\dagger \Psi_i e^{-ipx_i}. \end{aligned} \quad (3.23)$$

The creation and annihilation operators in position and momentum representation are connected via Fourier transformation

$$\begin{aligned}\psi_j^\dagger &= \frac{1}{\sqrt{V}} \sum_k e^{-ikx_j} a_k^\dagger, \\ \psi_j &= \frac{1}{\sqrt{V}} \sum_{k'} e^{ik'x_j} a_{k'},\end{aligned}\tag{3.24}$$

with momenta k and k' . Inserting these relations into eq. (3.23) yields

$$n_p = \int dx_j \sum_{k,k'} \frac{1}{V} a_k^\dagger a_{k'} e^{-ix_j(p+k-k')}.\tag{3.25}$$

We use the integral representation of the delta function

$$\int_0^V dx_j e^{-ix_j(p+k-k')} = V\delta(p+k-k').\tag{3.26}$$

Hence the density in eq. (3.25) becomes

$$\begin{aligned}n_p &= \frac{V}{V} \sum_{k,k'} a_k^\dagger a_{k'} \delta(p+k-k') \\ &= \sum_k a_k^\dagger a_{k+p}.\end{aligned}\tag{3.27}$$

Inserting the result into eq. (3.22), we obtain an expression for the real space density depending on creation and annihilation operators of the Fourier space

$$n_i = \sum_{p,k} \frac{1}{V} e^{ipx_i} a_k^\dagger a_{k+p}.\tag{3.28}$$

The particle in the well couples to the density at coordinate $x_i = 0$ like shown in Figure 3.1, hence the density becomes

$$n_i(x_i = 0) = \sum_{p,k} \frac{1}{V} a_k^\dagger a_{k+p}.\tag{3.29}$$

Since we are describing a Bose-Einstein-condensate, we are interested in the ground state with zero momentum, We therefore only consider Fourier components for which at least one operator has zero momentum. Since there are two indices in eq. (3.29), there are two ground state components

$$\begin{aligned}k = 0 : & \quad \sum_p \frac{1}{V} a_p^\dagger a_0 \\ k = -p : & \quad \sum_p \frac{1}{V} a_0^\dagger a_{-p}.\end{aligned}\tag{3.30}$$

After expanding the sum over momentum k in eq. (3.29), we hence obtain

$$\begin{aligned} n_i(x_i = 0) &= \frac{1}{V} a_0 \sum_p (a_p^\dagger + a_{-p}) \\ &= \frac{1}{V} a_0 \left(\sum_p a_p^\dagger + \sum_{p'} a_{-p'} \right). \end{aligned} \quad (3.31)$$

We redefine $p' = -p$ and arrive at

$$\begin{aligned} n_i(x_i = 0) &= \frac{1}{V} a_0 \left(\sum_p a_p^\dagger + \sum_p a_p \right) \\ &= \frac{a_0}{V} \sum_p (a_p + a_p^\dagger). \end{aligned} \quad (3.32)$$

The real space density is now expressed as a sum of creation and annihilation operators in momentum space. Inserting eq. (3.32) into the interaction term in eq. (3.21) yields

$$\begin{aligned} H_1^{\text{mic}} &= \frac{1}{2} g_{ab} \sigma_z (n_1(0) - n_2(0)) \\ &= \frac{1}{2} g_{ab} \sigma_z \frac{a_0}{V} \sum_p \left((a_{p1}^\dagger + a_{p1}) - (a_{p2}^\dagger + a_{p2}) \right) \\ &= \frac{1}{2} g_{ab} \sigma_z \frac{a_0}{V} \sum_p (a_{p1}^\dagger + a_{p1} - a_{p2}^\dagger - a_{p2}). \end{aligned} \quad (3.33)$$

In order to perform the mapping between the systems, the Hamiltonian has to be of the same form as the SB-Hamiltonian in eq. (2.19). This can be achieved by introducing the Bogoliubov transformation

$$\begin{aligned} a_p &= u_p b_p + v_{-p}^* b_{-p}^\dagger \\ a_p^\dagger &= u_p^* b_p^\dagger + v_{-p} b_{-p}. \end{aligned} \quad (3.34)$$

We then obtain for the interaction term in eq. (3.33)

$$\begin{aligned} H_1^{\text{mic}} &= \frac{1}{2} g_{ab} \sigma_z \frac{a_0}{V} \sum_p (u_{p1}^* b_{p1}^\dagger + v_{-p1} b_{-p1} + u_{p1} b_{p1} + v_{-p1}^* b_{-p1}^\dagger - u_{p2}^* b_{p2}^\dagger - v_{-p2} b_{-p2} - \\ &\quad - u_{p2} b_{p2} - v_{-p2}^* b_{-p2}^\dagger). \end{aligned} \quad (3.35)$$

As the bose tube 1 and the bose tube 2 are assumed to be totally identical in their physical properties we can set up some symmetry relations for the Bogoliubov coefficients

$$\begin{aligned} u_{p1} &= u_{p2} = u_p, & v_{-p1} &= v_{-p2} = v_{-p} \\ u_{p1}^* &= u_{p2}^* = u_p^*, & v_{-p1}^* &= v_{-p2}^* = v_{-p}^*. \end{aligned} \quad (3.36)$$

Applying these relations, eq. (3.35) reduces to

$$\begin{aligned}
H_1^{\text{mic}} &= \frac{1}{2} g_{\text{ab}} \sigma_z \frac{a_0}{V} \sum_p (u_p^* b_{p1}^\dagger + v_{-p} b_{-p1} + u_p b_{p1} + v_{-p}^* b_{-p1}^\dagger - u_p^* b_{p2}^\dagger - v_{-p} b_{-p2} - \\
&\quad - u_p b_{p2} - v_{-p}^* b_{-p2}^\dagger) \\
&= \frac{1}{2} g_{\text{ab}} \sigma_z \frac{a_0}{V} \left[\sum_p (u_p^* b_{p1}^\dagger + u_p b_{p1} - u_p^* b_{p2}^\dagger - u_p b_{p2}) \right. \\
&\quad \left. + \sum_{p'} (v_{-p'} b_{-p'1} + v_{-p'}^* b_{-p'1}^\dagger - v_{-p'} b_{-p'2} - v_{-p'}^* b_{-p'2}^\dagger) \right]. \quad (3.37)
\end{aligned}$$

As shown in the calculation of the density in (3.32) we can redefine the summation index $p' = -p$ and obtain

$$\begin{aligned}
H_1^{\text{mic}} &= \frac{1}{2} g_{\text{ab}} \sigma_z \frac{a_0}{V} \sum_p (u_p^* b_{p1}^\dagger + v_p b_{p1} + u_p b_{p1} + v_p^* b_{p1}^\dagger - u_p^* b_{p2}^\dagger - v_p b_{p2} - u_p b_{p2} - v_p^* b_{p2}^\dagger) \\
&= \frac{1}{2} g_{\text{ab}} \sigma_z \frac{a_0}{V} \sum_p (u_p^* (b_{p1}^\dagger - b_{p2}^\dagger) + v_p^* (b_{p1}^\dagger - b_{p2}^\dagger) + u_p (b_{p1} - b_{p2}) + v_p (b_{p1} - b_{p2})) \\
&= \frac{1}{2} g_{\text{ab}} \sigma_z \frac{a_0}{V} \sum_p (u_p^* + v_p^*) b_{p-}^\dagger + (v_p + u_p) b_{p-}. \quad (3.38)
\end{aligned}$$

To simplify the term above we introduce new, possibly non-normalized antisymmetric creation and annihilation operators

$$\begin{aligned}
b_{p-}^\dagger &= A (b_{p1}^\dagger - b_{p2}^\dagger), \\
b_{p-} &= A (b_{p1} - b_{p2}). \quad (3.39)
\end{aligned}$$

We still have to consider the normalization to make sure, we are dealing with bosonic operators, which means they have to satisfy the bosonic commutation relation

$$\begin{aligned}
[b_{p-}, b_{p-}^\dagger] &= A^2 [b_{p1} - b_{p2}, b_{p1}^\dagger - b_{p2}^\dagger] \\
&= A^2 [b_{p1}, b_{p1}^\dagger - b_{p2}^\dagger] - A^2 [b_{p2}, b_{p1}^\dagger - b_{p2}^\dagger] \\
&= A^2 \underbrace{[b_{p1}, b_{p1}^\dagger]}_{=1} - A^2 \underbrace{[b_{p1}, b_{p2}^\dagger]}_{=0} - A^2 \left(\underbrace{[b_{p2}, b_{p1}^\dagger]}_{=0} - \underbrace{[b_{p2}, b_{p2}^\dagger]}_{=1} \right) \\
&= (1 - 0 - 0 + 1)A^2 = 2A^2 \quad (3.40)
\end{aligned}$$

We then obtain for the normalization factor

$$2A^2 = 1 \Rightarrow A = \frac{1}{\sqrt{2}} \quad (3.41)$$

Where the fact has been used, that the Bogoliubov operators fulfill the bosonic commutation relation $[b_i, b_j^\dagger] = \delta_{ij}$. With the result of eq. (3.41) the antisymmetric operators of eq. (3.39) read

$$\begin{aligned}
\sqrt{2} b_{p-} &= (b_{p1} - b_{p2}), \\
\sqrt{2} b_{p-}^\dagger &= (b_{p1}^\dagger - b_{p2}^\dagger). \quad (3.42)
\end{aligned}$$

Inserting these results into eq. (3.38) yields

$$H_I^{\text{mic}} = \frac{1}{2} g_{ab} \sigma_z \frac{a_0 \sqrt{2}}{V} \sum_p \left((u_p^* + v_p^*) b_{p-}^\dagger + (v_p + u_p) b_{p-} \right). \quad (3.43)$$

Assuming that u_p and v_p are real numbers, we arrive at

$$H_I^{\text{mic}} = \frac{1}{2} g_{ab} \sigma_z \frac{a_0 \sqrt{2}}{V} \sum_p (v_p + u_p) \left(b_{p-}^\dagger + b_{p-} \right). \quad (3.44)$$

We achieved that the Hamiltonian has the same form as the one in eq. (2.19). Summarizing the result of this subsection the microscopic Hamiltonian reads

$$\begin{aligned} H^{\text{mic}} = & -J\sigma_x + E_{01} + E_{02} + \sum_p \epsilon(p) b_{p1}^\dagger b_{p1} + \sum_p \epsilon(p) b_{p2}^\dagger b_{p2} + \\ & + \frac{1}{2} g_{ab} \sigma_z \frac{a_0 \sqrt{2}}{V} \sum_p (v_p + u_p) \left(b_{p-}^\dagger + b_{p-} \right). \end{aligned} \quad (3.45)$$

The coupling constant

The comparison of the Hamiltonians of eq. (2.19) and (3.44)

$$\begin{aligned} H_I^{\text{SB}} &= -\frac{1}{2} \sigma_z q_0 \sum_\alpha \lambda_\alpha (b_\alpha + b_\alpha^\dagger), \\ H_I^{\text{mic}} &= \frac{1}{2} g_{ab} \sigma_z \frac{a_0 \sqrt{2}}{V} \sum_p (v_p + u_p) \left(b_{p-}^\dagger + b_{p-} \right), \end{aligned} \quad (3.46)$$

yields

$$\lambda_\alpha = -\frac{a_0 \sqrt{2} g_{ab}}{V q_0} (v_p + u_p). \quad (3.47)$$

Using eq. (2.20), we obtain

$$\begin{aligned} c_\alpha &= -\frac{\sqrt{2} a_0 g_{ab}}{V q_0} \sqrt{\frac{2 m_\alpha \omega_\alpha}{\hbar}} (v_p + u_p) \\ &= -\frac{2 a_0 g_{ab}}{V q_0} \sqrt{\frac{m_\alpha \omega_\alpha}{\hbar}} (v_p + u_p). \end{aligned} \quad (3.48)$$

As mentioned before the indices can be interchanged and the coupling constant becomes

$$c(p) = -\frac{2 a_0 g_{ab}}{V q_0} \sqrt{\frac{m(p) \omega(p)}{\hbar}} (v_p + u_p). \quad (3.49)$$

As the coupling constant enters the spectral function squared, we are only interested in the squared sum of the Bogoliubov coefficients

$$\begin{aligned}
(u_p + v_p)^2 &= \left(\sqrt{\frac{p^2}{2m} + gn} + \frac{1}{2} - \sqrt{\frac{p^2}{2m} + gn} - \frac{1}{2} \right)^2 \\
&= \frac{p^2}{2m} + gn + \frac{1}{2} - 2 \sqrt{\left(\frac{p^2}{2m} + gn + \frac{1}{2} \right) \left(\frac{p^2}{2m} + gn - \frac{1}{2} \right)} + \frac{p^2}{2m} + gn - \frac{1}{2} \\
&= \frac{p^2}{2m} + gn - \sqrt{\left(\frac{p^2}{2m} + gn \right)^2 - 1} \\
&= \frac{p^2}{2m} + gn - \sqrt{\frac{\left(\frac{p^2}{2m} + gn \right)^2 - \epsilon(p)^2}{\epsilon(p)^2}}.
\end{aligned} \tag{3.50}$$

The Bogoliubov dispersion relation $\epsilon(p)$ reads

$$\begin{aligned}
\epsilon(p)^2 &= \frac{gnp^2}{m} + \left(\frac{p^2}{2m} \right)^2 \\
&= \left(\frac{p^2}{2m} + gn \right)^2 - (gn)^2.
\end{aligned} \tag{3.51}$$

Hence eq. (3.50) can be simplified as

$$\begin{aligned}
(u_p + v_p)^2 &= \frac{\frac{p^2}{2m} + gn}{\epsilon(p)} - \sqrt{\frac{\left(\frac{p^2}{2m} + gn \right)^2 - \left(\frac{p^2}{2m} + gn \right)^2 - (gn)^2}{\epsilon(p)^2}} \\
&= \frac{p^2}{2m\epsilon(p)}.
\end{aligned} \tag{3.52}$$

If we square eq. (3.49) and then insert the expression into eq. (3.52), we obtain for the coupling constant

$$c(p)^2 = \frac{2a_0^2 g_{ab}^2 m(p) \omega(p)}{V^2 q_0^2 \hbar} \frac{p^2}{m\epsilon(p)}, \tag{3.53}$$

where m is the mass of a boson and $m(p)$ is the mass of the p -th harmonic oscillator and hence a parameter. The Bogoliubov dispersion relation $\epsilon(p)$ is given as

$$\begin{aligned}
\epsilon(p) &= \sqrt{\frac{p^4}{4m^2} + \frac{p^2 gn}{m}} = \sqrt{\frac{p^2 gn}{m} \left(\frac{p^2}{4mgn} + 1 \right)} \\
&= |p| \sqrt{\frac{gn}{m}} \sqrt{1 + \frac{p^2}{4mgn}}.
\end{aligned} \tag{3.54}$$

Since we describe a BEC, we are only interested in the dispersion relation in the limit of small momenta. The expansion of the square root reads

$$\sqrt{1+x} \approx 1 + \frac{1}{2}x - \frac{1}{8}x^2 + \dots \tag{3.55}$$

Applying the above equation in first order the dispersion relation in eq. (3.54) has a phonon-like form

$$\epsilon(p) \approx |p| \sqrt{\frac{gn}{m}} = |p| v_s, \quad (3.56)$$

where v_s is the sound velocity

$$v_s = \sqrt{\frac{gn}{m}}. \quad (3.57)$$

Inserting the result of the expansion in eq. (3.56) into eq. (3.53) yields

$$c(p)^2 = \frac{2a_0^2 g_{ab}^2 \omega(p) m(p)}{V^2 q_0^2 \hbar} \frac{|p|}{mv_s} \quad (3.58)$$

We arrived at an expression for the coupling constant of the microscopic double well.

The spectral function

The spectral function for the Caldeira Leggett model reads

$$J(\omega) = \frac{\pi}{2} \sum_{\alpha} \left(\frac{c_{\alpha}^2}{m_{\alpha} \omega_{\alpha}} \right) \delta(\omega - \omega_{\alpha}). \quad (3.59)$$

We can replace the sum by an integral in the limes

$$\lim_{n \rightarrow \infty} \sum_{i=1}^n f(p_i) \Delta p_{i-1} = \int f(p) dp. \quad (3.60)$$

The distance is given as

$$\Delta p_0 = \Delta p_1 = \Delta p_2 = \dots = \Delta p_{n-1} = \frac{2\pi\hbar}{V}. \quad (3.61)$$

Inserting the above relation into eq. (3.60) yields

$$\lim_{n \rightarrow \infty} \sum_{i=1}^n f(p_i) = \frac{V}{2\pi\hbar} \int f(p) dp. \quad (3.62)$$

We then arrive at the integral expression of the spectral function

$$J(\omega) = \frac{V}{4\hbar} \int dp \frac{c^2(p)}{m(p)\omega(p)} \delta(\omega - \omega(p)). \quad (3.63)$$

Inserting the result for the coupling constant of eq. (3.58), yields

$$J(\omega) = \frac{1}{2\hbar^2} \int dp \frac{a_0^2 g_{ab}^2 |p|}{V q_0^2 m v_s} \delta(\omega - \omega(p)). \quad (3.64)$$

The result of the environment mapping in eq. (3.19) gives the relation between the dispersion relation and the frequency

$$\omega(p) = \frac{\epsilon(p)}{\hbar} = \frac{|p| v_s}{\hbar}, \quad (3.65)$$

where we inserted the small momentum expansion of eq. (3.56) for the dispersion relation. After inserting the above result into the delta function of eq. (3.64) the integral can be evaluated

$$\begin{aligned}
J(\omega) &= \frac{1}{2\hbar^2} \int_{-\infty}^{\infty} d\rho \frac{a_0^2 g_{ab}^2}{Vq_0^2} \frac{|\rho|}{mv_s} \delta\left(\omega - \frac{|\rho| v_s}{\hbar}\right) \\
&= \frac{1}{\hbar^2} \int_0^{\infty} d\rho \frac{a_0^2 g_{ab}^2}{Vq_0^2} \frac{\rho}{mv_s} \delta\left(\omega - \frac{\rho v_s}{\hbar}\right) \\
&= \frac{a_0^2 g_{ab}^2}{Vq_0^2 m v_s^3} \omega.
\end{aligned} \tag{3.66}$$

For the sound velocity in the denominator we write

$$v_s^2 = \frac{gn}{m}. \tag{3.67}$$

In the case of a BEC the zero momentum operator a_0 is the c-number $\sqrt{N_0}$, where N_0 is the number of bosons in the ground state. Due to the interactions between the particles in the condensate, not all of them enter the ground state, so that the total number N of particles does not exactly equal the number N_0 of particles in the ground state (quantum depletion). Hence the ground state density n_0 or density of the condensate is

$$n_0 = \frac{a_0^2}{V} = \frac{N_0}{V} \neq \frac{N}{V} = n, \tag{3.68}$$

with dimension one over length. Inserting eq. (3.67) and (3.68) into eq. (3.66) yields the spectral function

$$J(\omega) = \frac{n_0 g_{ab}^2}{ng} \frac{1}{q_0^2 v_s} \omega, \tag{3.69}$$

where g_{ab} is the collision parameter between a particle in the condensate and the particle in the well, whereas g is the collision parameter of two particles in the condensate. The spectral function for the microscopic system is proportional to the frequency, thus we have ohmic dissipation.

Dissipation coefficient and coupling strength of the microscopic double well

In the case of ohmic dissipation the spectral function can be written as

$$J(\omega) = \eta\omega, \tag{3.70}$$

where η is the dissipation coefficient. From eq. (3.69) we can therefore read off the the dissipation coefficient

$$\eta = \frac{n_0 g_{ab}^2}{ng} \frac{1}{q_0^2 v_s}. \tag{3.71}$$

The dissipation coefficient is of dimension action over length squared and the spectral function has the dimension mass times frequency squared. The dissipation coefficient can be converted

into the dimensionless coupling strength

$$\begin{aligned}\alpha &= \eta \frac{q_0^2}{2\pi\hbar} \\ &= \frac{1}{2\pi} \frac{n_0 g_{ab}^2}{ng} \frac{1}{\hbar v_s}.\end{aligned}\quad (3.72)$$

A little auxiliary calculation helps to simplify the coupling parameter

$$\frac{1}{\hbar v_s} = \sqrt{\frac{m}{gn\hbar^2}} = \frac{1}{g} \sqrt{\frac{gm}{n\hbar^2}}.\quad (3.73)$$

Then the coupling strength in eq. (3.72) becomes

$$\begin{aligned}\alpha &= \frac{1}{2\pi} \frac{n_0 g_{ab}^2}{ng} \frac{1}{g} \sqrt{\frac{gm}{n\hbar^2}} \\ &= \frac{1}{2\pi} \frac{n_0 g_{ab}^2}{ng^2} \sqrt{\gamma}.\end{aligned}\quad (3.74)$$

The quantity γ expresses the ratio between the interaction and the kinetic energy of a particle in the condensate

$$\gamma = \frac{E_{int}}{E_{kin}} = \frac{gm}{n\hbar^2}.\quad (3.75)$$

The energies have been approximated as follows

$$E_{kin} \approx \frac{\hbar^2 k^2}{m} \stackrel{1D}{=} \frac{\hbar^2 n^2}{m}, \quad E_{int} \stackrel{1D}{=} gn.\quad (3.76)$$

In the case of a one dimensional condensate the density n and the wavenumber k have the dimension one over length and we are allowed to replace the wavenumber by the density. The coupling strength α of the particle and the tubes is strong, if the interactions between the bosons in the tubes are strong.

3.4 Microscopic lattice

We expand the microscopic double well and consider a particle tunneling between the neighboring minima of a periodic potential. Each well j is overlaid with a bose tube of density n_j . We are going to set up the microscopic Hamiltonian and determine the physical parameters of the system.

3.4.1 Derivation of the microscopic Hamiltonian describing the lattice

By expanding the double well to a lattice, the TSS becomes a multi state system. In order to describe the lattice we introduce the annihilation and creation operators c_j and c_j^\dagger of a particle on site j . In the microscopic multi state system the particle in the j -th well couples exclusively to the density $n(0)_j$ of the j -th bose tube, see Figure 3.2. Like in the case of the double well the bose

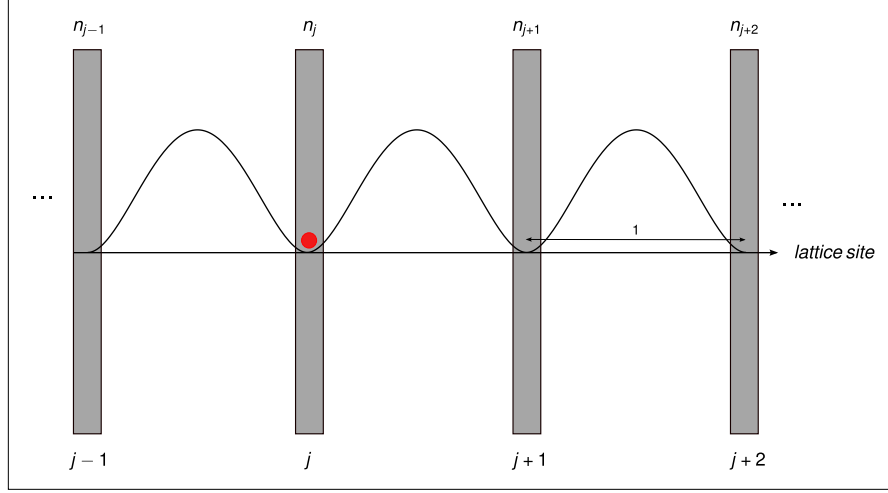


Figure 3.2 The microscopic lattice. The particle in the well j couples to the density of the j -th bose tube.

tubes are described by the Bogoliubov theory of a weakly interacting BEC. The Hamiltonian for the microscopic lattice thus reads

$$H^{\text{mic}} = -J \sum_{\langle i,j \rangle} c_i^\dagger c_j + \sum_{p,j} \epsilon(p) b_{pj}^\dagger b_{pj} + \sum_j U_j c_j^\dagger c_j. \quad (3.77)$$

The first term describes the tunneling between two neighboring lattice sites $\langle i,j \rangle$ with the hopping matrix element J . The second term describes the environment, where b_{pj} and b_{pj}^\dagger are the bosonic Bogoliubov annihilation and creation operators of the j -th bose tube. The last term describes the coupling. The interaction energy for the coupling to the j -th tube is given as

$$\begin{aligned} U_j &= g_{ab} n_j(0) \\ &= g_{ab} \frac{a_0}{V} \sum_{p,j} (a_{pj} + a_{pj}^\dagger), \end{aligned} \quad (3.78)$$

where we used the result of eq. (3.32) to express the density by creation and annihilation operators. Analogous to the case of the double well, we can argue that all j bose tubes are identical. Hence we can use the symmetry relations of eq. (3.36). Assuming that the coefficients are real numbers yields for the Bogoliubov transformation

$$\begin{aligned} a_{pj} &= u_p b_{pj} + v_{-p} b_{-pj}^\dagger \\ a_{pj}^\dagger &= u_p b_{pj}^\dagger + v_{-p} b_{-pj}. \end{aligned} \quad (3.79)$$

Then the interaction energy becomes

$$\begin{aligned} U_j &= g_{ab} \frac{a_0}{V} \sum_{p,j} (u_p b_{pj}^\dagger + u_p b_{pj}) + \sum_{p',j} (v_{-p'} b_{-p'j}^\dagger + v_{-p'} b_{-p'j}) \\ &\stackrel{p'=-p}{=} g_{ab} \frac{a_0}{V} \sum_{p,j} (u_p b_{pj} + v_p b_{pj}^\dagger + u_p b_{pj}^\dagger + v_p b_{pj}) \end{aligned} \quad (3.80)$$

$$\begin{aligned}
&= g_{ab} \frac{a_0}{V} \sum_{\rho,j} (u_\rho + v_\rho) b_{\rho j}^\dagger + (u_\rho + v_\rho) b_{\rho j} \\
&= g_{ab} \frac{a_0}{V} \sum_{\rho,j} \left((u_\rho + v_\rho) (b_{\rho j}^\dagger + b_{\rho j}) \right). \tag{3.81}
\end{aligned}$$

Inserting the above result into eq. (3.77) yields

$$H^{\text{mic}} = -J \sum_{i,j} c_i^\dagger c_j + \sum_{\rho,j} \epsilon(\rho) b_{\rho j}^\dagger b_{\rho j} + \sum_{\rho,j} g_{ab} \frac{a_0}{V} (u_\rho + v_\rho) (b_{\rho j}^\dagger + b_{\rho j}) c_j^\dagger c_j. \tag{3.82}$$

3.4.2 Physical parameters of the microscopic lattice

The interaction term of eq. (3.82) leads to

$$\lambda(\rho)_{\text{lattice}} = \frac{g_{ab} a_0}{V} (u_\rho + v_\rho). \tag{3.83}$$

Since there is no dependence on the index j , the coupling between the particle and each bose tube is identical. The structure of the above expression coincides with the result of eq. (3.47) for the microscopic double well, if the TB lattice constant q_0 is chosen to be equal one, as shown in Figure 3.2. Still both expressions differ by $\sqrt{2}$. Taking this factor into account we might define, analogous to the double well, the dissipation coefficient and the coupling strenght of the lattice, respectively

$$\begin{aligned}
\eta_{\text{lattice}} &= \frac{n_0 g_{ab}^2}{2ng} \frac{1}{v_s}, \\
\alpha_{\text{lattice}} &= \eta_{\text{lattice}} \frac{1}{2\pi\hbar} = \frac{1}{4\pi} \frac{n_0 g_{ab}^2}{ng} \frac{1}{\hbar v_s} = \frac{1}{4\pi} \frac{n_0 g_{ab}^2}{ng^2} \sqrt{\gamma}. \tag{3.84}
\end{aligned}$$

The comparison with the coupling strength of the microscopic double well in eq. (3.74) yields

$$\alpha_{\text{double}}^{\text{mic}} = 2\alpha_{\text{lattice}}^{\text{mic}}. \tag{3.85}$$

We must conclude that the coupling of the expanded system differs from the double well. This originates from the normalization factor $1/\sqrt{2}$ in eq. (3.41) of the antisymmetric annihilation and creation operators. Form a physical point of view, the difference therefore arises, because the particle in the double well couples to the antisymmetric mode ($n_1 - n_2$), but in the case of the lattice it couples exclusively to the tube n_j corresponding to the well j .

Effective action

4.1 Density matrix of the reduced system

We follow the calculation in [8]. Our goal is to derive a form for the density matrix that only depends on the coordinate q of the particle, so we have to eliminate the explicit dependence on the coordinates \mathbf{x} of the environment. The calculation is rather extensive, so it is a good idea to have a short survey of the important considerations of the calculation. The connection between the imaginary time path integral formalism and statistical mechanics was shown in section 2.4. In the Caldeira Legget model the density matrix for the total system is given by

$$\begin{aligned} \rho &= \frac{1}{Z_{\text{tot}}} \int \mathcal{D}[q(\tau)] \int \mathcal{D}[\mathbf{x}(\tau)] e^{-\frac{1}{\hbar}(S_S(q) + S_I(q, \mathbf{x}) + S_E(\mathbf{x}))} \\ &= \frac{1}{Z_{\text{tot}}} \int \mathcal{D}[q(\tau)] \int \mathcal{D}[\mathbf{x}(\tau)] e^{-\frac{1}{\hbar} S_S(q)} e^{-\frac{1}{\hbar}(S_I(q, \mathbf{x}) + S_E(\mathbf{x}))}. \end{aligned} \quad (4.1)$$

The coordinates of the harmonic oscillators can be divided into a classical part $\bar{\mathbf{x}}$ and a fluctuating part \mathbf{y} describing the quantum mechanics

$$\mathbf{x} = \mathbf{y} + \bar{\mathbf{x}}. \quad (4.2)$$

Applying the coordinate transformation of eq. (4.2) to the density matrix gives

$$\rho = \frac{1}{Z_{\text{tot}}} \int \mathcal{D}[q(\tau)] \int \mathcal{D}[\mathbf{y}(\tau)] e^{-\frac{1}{\hbar} S_S(q)} e^{-\frac{1}{\hbar}(S_{\text{int}}(\bar{\mathbf{x}}) + S_E(\mathbf{y}))}. \quad (4.3)$$

With the help of the coordinate transformation the interaction term and the environment term of the action decouple. This is only possible because the coupling between the environment and the particle is assumed to be linear. As a consequence we are able to rearrange the density matrix as following

$$\rho = \frac{1}{Z} \int \mathcal{D}[q(\tau)] e^{-\frac{1}{\hbar}(S_S(q) + S_{\text{int}}(\bar{\mathbf{x}}))} \underbrace{\frac{1}{Z_E} \int \mathcal{D}[\mathbf{y}(\tau)] e^{-\frac{1}{\hbar} S_E(\mathbf{y})}}_{Z_E}, \quad (4.4)$$

where Z is the partition function of the open damped system, also named reduced system. The partition function Z_E of the environment is exactly canceled by the path over the quantum

fluctuations, so the density matrix of the reduced system becomes

$$\rho = \frac{1}{Z} \int \mathcal{D}[q(\tau)] e^{-\frac{1}{\hbar}(S_S(q) + S_{\text{int}}(\bar{x}))}. \quad (4.5)$$

Since the classical part \bar{x} of the harmonic oscillator coordinates can be related to the coordinate q of the particle by solving the classical equations of motion, we obtain a reduced density matrix that exclusively depends on the coordinate q

$$\rho = \frac{1}{Z} \int \mathcal{D}[q(\tau)] e^{-\frac{1}{\hbar}(S_S(q) + S_{\text{int}}(q))} = \frac{1}{Z} \int \mathcal{D}[q(\tau)] e^{-\frac{1}{\hbar} S_{\text{eff}}(q)}. \quad (4.6)$$

The effective formulation of the system coupled to the environment does not explicitly depend on the environment. The influence of the environment is implicitly incorporated in the influence action.

4.1.1 Derivation of the influence action

To give more insight in the derivation of the influence action we reproduce the most important steps of the calculation shown in [8]. The influence action only depends on the coordinate q of the particle. Hence we have to consider the terms of the Lagrangian, that depends on the coordinate x_α of the environment

$$L_E + L_I + \text{counterterm} = \frac{1}{2} \sum_{\alpha} m_{\alpha} (\dot{x}_{\alpha}^2 + \omega_{\alpha}^2 x_{\alpha}^2) - \sum_{\alpha} c_{\alpha} x_{\alpha} q + \sum_{\alpha} \frac{1}{2} \frac{c_{\alpha}^2 q^2}{m_{\alpha} \omega_{\alpha}^2}. \quad (4.7)$$

The discrete Fourier transformation is given by

$$\begin{aligned} x_{\alpha}(\tau) &= \frac{1}{\hbar\beta} \sum_n x_{\alpha n} e^{i\nu_n \tau}, \\ q(\tau) &= \frac{1}{\hbar\beta} \sum_n q_n e^{i\nu_n \tau}, \end{aligned} \quad (4.8)$$

with the the Matsubara frequency for bosons

$$\nu_n = \frac{2\pi n}{\hbar\beta}. \quad (4.9)$$

Inserting the Fourier transformation of eq. (4.8) the action can be rewritten as

$$\begin{aligned} S_{E,I} &= \int_0^{\hbar\beta} d\tau \left(\frac{1}{2\hbar^2\beta^2} \sum_{\alpha, n, n'} m_{\alpha} \left(\partial_{\tau} x_{\alpha n} e^{i\nu_n \tau} \partial_{\tau} x_{\alpha n'} e^{i\nu_{n'} \tau} + \omega_{\alpha}^2 x_{\alpha n} e^{i\nu_n \tau} x_{\alpha n'} e^{i\nu_{n'} \tau} \right) \right) \\ &\quad - \int_0^{\hbar\beta} d\tau \left(\frac{1}{\hbar^2\beta^2} \sum_{\alpha, n, n'} c_{\alpha} x_{\alpha n} e^{i\nu_n \tau} q_{n'} e^{i\nu_{n'} \tau} \right) \\ &\quad + \int_0^{\hbar\beta} d\tau \left(\sum_{\alpha, n, n'} \frac{1}{2\hbar^2\beta^2} \frac{c_{\alpha}^2 q_n e^{i\nu_n \tau} q_{n'} e^{i\nu_{n'} \tau}}{m_{\alpha} \omega_{\alpha}^2} \right) \end{aligned} \quad (4.10)$$

$$\begin{aligned}
S_{E,I} = & \int_0^{\hbar\beta} d\tau \left(\frac{1}{2\hbar^2\beta^2} \sum_{\alpha,n,n'} m_\alpha \left(x_{\alpha n} x_{\alpha n'} i^2 \nu_n \nu_{n'} e^{-i(-\nu_n - \nu_{n'})\tau} + \omega_\alpha^2 x_{\alpha n} x_{\alpha n'} e^{-i(-\nu_n - \nu_{n'})\tau} \right) \right) \\
& - \int_0^{\hbar\beta} d\tau \left(\frac{1}{\hbar^2\beta^2} \sum_{\alpha,n,n'} c_\alpha x_{\alpha n} q_{n'} e^{-i(-\nu_n - \nu_{n'})\tau} \right) \\
& + \int_0^{\hbar\beta} d\tau \left(\sum_{\alpha,n,n'} \frac{1}{2\hbar^2\beta^2} \frac{c_\alpha^2 q_n q_{n'}}{m_\alpha \omega_\alpha^2} e^{-i(-\nu_n - \nu_{n'})\tau} \right). \tag{4.11}
\end{aligned}$$

If the coordinates x_α and the coordinate q are real, the Fourier components fulfill

$$-\nu_n = \nu_{-n}, \quad x_{\alpha n} = x_{\alpha(-n)}^*, \quad q_n = q_{-n}^*. \tag{4.12}$$

The delta function is given as

$$\int_0^{\hbar\beta} d\tau e^{-i(\nu_{-n} - \nu_{n'})\tau} = \hbar\beta \delta(\nu_{-n} - \nu_{n'}). \tag{4.13}$$

Applying the above relations simplifies the expression for the action

$$\begin{aligned}
S_{E,I} = & \frac{1}{2\hbar\beta} \sum_{\alpha,n,n'} m_\alpha \left(x_{\alpha(-n)}^* x_{\alpha n'} i^2 \nu_n \nu_{n'} \delta(\nu_{-n} - \nu_{n'}) + \omega_\alpha^2 x_{\alpha(-n)}^* x_{\alpha n'} \delta(\nu_{-n} - \nu_{n'}) \right) \\
& - \frac{1}{\hbar\beta} \sum_{\alpha,n,n'} c_\alpha x_{\alpha(-n)}^* q_{n'} \delta(\nu_{-n} - \nu_{n'}) + \sum_{\alpha,n,n'} \frac{1}{2\hbar\beta} \frac{c_\alpha^2 q_{-n}^* q_{n'}}{m_\alpha \omega_\alpha^2} \delta(\nu_{-n} - \nu_{n'}). \tag{4.14}
\end{aligned}$$

We can now perform the summation over n . The delta function leads to the following condition

$$\nu_{-n} = \nu_{n'} \Rightarrow -n = n'. \tag{4.15}$$

We then obtain

$$\begin{aligned}
S_{E,I} = & \frac{1}{2\hbar\beta} \sum_{\alpha,n'} m_\alpha \left(x_{\alpha n'}^* x_{\alpha n'} i^2 \underbrace{\nu_{-n'}}_{=(-\nu_{n'})} \nu_{n'} + \omega_\alpha^2 x_{\alpha n'}^* x_{\alpha n'} \right) - \frac{1}{\hbar\beta} \sum_{\alpha,n'} c_\alpha x_{\alpha n'}^* q_{n'} \\
& + \sum_{\alpha,n'} \frac{1}{2\hbar\beta} \frac{c_\alpha^2 q_{n'}^* q_{n'}}{m_\alpha \omega_\alpha^2} \\
= & \frac{1}{2\hbar\beta} \sum_{\alpha,n'} m_\alpha \left(|x_{\alpha n'}|^2 \nu_{n'}^2 + \omega_\alpha^2 |x_{\alpha n'}|^2 \right) - \frac{1}{\hbar\beta} \sum_{\alpha,n'} c_\alpha x_{\alpha n'}^* q_{n'} + \sum_{\alpha,n'} \frac{1}{2\hbar\beta} \frac{c_\alpha^2 |q_{n'}|^2}{m_\alpha \omega_\alpha^2}. \tag{4.16}
\end{aligned}$$

In the last expression the index n' can be replaced by n . We have mentioned in the previous section that a coordinate transformation as in eq. (4.2) is necessary to decouple the action. The fluctuating term will be canceled as shown in eq. (4.4). Hence we are only interested in the classical part

$$S_{\text{infl}} = \frac{M}{2} \frac{1}{\hbar\beta} \sum_n \xi_n |q_n|^2 \tag{4.17}$$

where M is the mass of the particle in the potential and

$$\xi_n = \frac{1}{M} \sum_{\alpha} \frac{c_{\alpha}^2}{m_{\alpha} \omega_{\alpha}^2} \frac{\nu_n^2}{(\nu_n^2 + \omega_{\alpha}^2)}. \quad (4.18)$$

It is convenient to express the above equation in terms of the spectral function

$$\xi_n = \frac{1}{M} \sum_{\alpha} \frac{c_{\alpha}^2}{m_{\alpha} \omega_{\alpha}^2} \frac{\nu_n^2}{(\nu_n^2 + \omega_{\alpha}^2)} = \frac{2}{M\pi} \int_0^{\infty} d\omega \frac{J(\omega)}{\omega} \frac{\nu_n^2}{(\nu_n^2 + \omega^2)}. \quad (4.19)$$

This can be seen considering

$$\frac{2}{M\pi} \int_0^{\infty} d\omega \frac{J(\omega)}{\omega} \frac{\nu_n^2}{(\nu_n^2 + \omega^2)}. \quad (4.20)$$

Employing the definition of the spectral function

$$J(\omega) = \frac{\pi}{2} \sum_{\alpha} \frac{c_{\alpha}^2}{m_{\alpha} \omega_{\alpha}} \delta(\omega - \omega_{\alpha}), \quad (4.21)$$

eq. (4.20) can be written as

$$\begin{aligned} & \frac{1}{M} \int_0^{\infty} d\omega \sum_{\alpha} \frac{c_{\alpha}^2}{m_{\alpha} \omega_{\alpha}} \frac{1}{\omega} \frac{\nu_n^2}{(\nu_n^2 + \omega^2)} \delta(\omega - \omega_{\alpha}) \\ &= \frac{1}{M} \sum_{\alpha} \frac{c_{\alpha}^2}{m_{\alpha} \omega_{\alpha}^2} \frac{\nu_n^2}{(\nu_n^2 + \omega_{\alpha}^2)}. \end{aligned} \quad (4.22)$$

The above expression coincides with eq. (4.18). Hence the influence action of eq. (4.17) becomes

$$S_{\text{infl}} = \frac{1}{\pi} \frac{1}{\hbar\beta} \sum_n \int_0^{\infty} d\omega \frac{J(\omega)}{\omega} \frac{\nu_n^2}{(\nu_n^2 + \omega^2)} |q_n|^2. \quad (4.23)$$

In the case of ohmic dissipation the spectral function reads

$$J(\omega) = \eta\omega, \quad (4.24)$$

where η is the dissipation coefficient. Then eq. (4.23) can be written as

$$\begin{aligned} S_{\text{infl}} &= \frac{1}{\pi} \frac{1}{\hbar\beta} \sum_n \eta \underbrace{\int_0^{\infty} d\omega \frac{\nu_n^2}{(\nu_n^2 + \omega^2)}}_{\frac{\pi}{2} |\nu_n|} |q_n|^2 \\ &= \frac{1}{2} \frac{1}{\hbar\beta} \sum_n \eta |\nu_n| |q_n|^2 \end{aligned} \quad (4.25)$$

In order to rewrite the influence action as an integral expression we use the relation of eq. (3.60), that we applied to the spectral function in section 3.3.3

$$\lim_{n \rightarrow \infty} \sum_{i=1}^n f(\nu_i) \Delta \nu_{i-1} = \int f(\nu) d\nu, \quad (4.26)$$

where the interval is given as

$$\Delta \nu_0 = \Delta \nu_1 = \Delta \nu_2 = \dots = \Delta \nu_{n-1} = \frac{2\pi}{\hbar\beta}. \quad (4.27)$$

In the limit $n \rightarrow \infty$ the frequency interval $\Delta \nu$ becomes very small and we therefore consider the limit $\beta \rightarrow \infty$. Hence the integral formulation of the influence action in eq. (4.25) is obtained for zero temperature and reads

$$\begin{aligned} S_{\text{infl}} &= \frac{1}{2} \frac{1}{\hbar\beta} \frac{\hbar\beta}{2\pi} \int d\nu \eta |\nu| |q(\nu)|^2 \\ &= \frac{\eta}{4\pi} \int d\nu |\nu| |q(\nu)|^2 = \frac{\eta}{4\pi} \int d\nu |\nu| q(\nu) q^*(\nu). \end{aligned} \quad (4.28)$$

To get the influence action of eq. (4.17) back in real space, we insert

$$\begin{aligned} q(\nu) &= \int d\tau q(\tau) e^{-i\nu\tau}, \\ q^*(\nu) &= \int d\tau q(\tau) e^{i\nu\tau}, \end{aligned} \quad (4.29)$$

and obtain

$$S_{\text{infl}} = \frac{\eta}{4\pi} \int d\tau \int d\tau' q(\tau') q(\tau) \int d\nu |\nu| e^{i\nu(\tau-\tau')}. \quad (4.30)$$

We calculate the Fourier transformation of $|\nu|$ with $\tau - \tau' = \tilde{\tau}$

$$\begin{aligned} \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} |\nu| e^{i\nu\tilde{\tau}} &= \int_{-\infty}^0 \frac{d\nu}{2\pi} \underbrace{(-\nu) e^{i\nu\tilde{\tau}}}_{-\frac{1}{i} \partial_{\tilde{\tau}} e^{i\nu\tilde{\tau}}} + \int_0^{\infty} \frac{d\nu}{2\pi} \underbrace{\nu e^{i\nu\tilde{\tau}}}_{\frac{1}{i} \partial_{\tilde{\tau}} e^{i\nu\tilde{\tau}}} \\ &= \frac{\partial_{\tilde{\tau}}}{2\pi i} \left(\int_{-\infty}^0 d\nu (-e^{i\nu\tilde{\tau}}) + \int_0^{\infty} d\nu e^{i\nu\tilde{\tau}} \right) \\ &= \frac{\partial_{\tilde{\tau}}}{2\pi i} \left(\left[-\frac{1}{i\tilde{\tau}} e^{i\nu\tilde{\tau}} \right]_{-\infty}^0 + \left[-\frac{1}{i\tilde{\tau}} e^{i\nu\tilde{\tau}} \right]_0^{\infty} \right) \\ &= \frac{\partial_{\tilde{\tau}}}{2\pi i} \left(\frac{2i}{\tilde{\tau}} - i \underbrace{\lim_{\tilde{\tau} \rightarrow -\infty} \frac{1}{\tilde{\tau}} e^{i\nu\tilde{\tau}}}_{=0} - i \underbrace{\lim_{\tilde{\tau} \rightarrow \infty} \frac{1}{\tilde{\tau}} e^{i\nu\tilde{\tau}}}_{=0} \right) \\ &= \frac{1}{\pi} \partial_{\tilde{\tau}} \frac{1}{\tilde{\tau}} = -\frac{1}{\pi} \frac{1}{\tilde{\tau}^2} = -\frac{1}{\pi} \frac{1}{(\tau - \tau')^2}. \end{aligned} \quad (4.31)$$

Then eq. (4.30) becomes

$$S_{\text{infl}} = -\frac{\eta}{2\pi} \int d\tau \int d\tau' \frac{q(\tau')q(\tau)}{(\tau - \tau')^2}. \quad (4.32)$$

The influence action does not change, if τ and τ' are interchanged, hence it is symmetric in both variables. It is convenient to rewrite the above expression, we therefore consider

$$q(\tau)q(\tau') = \frac{1}{2} \left(q^2(\tau) + q^2(\tau') - (q(\tau) - q(\tau'))^2 \right). \quad (4.33)$$

Due to symmetry considerations the terms only depending on τ or τ' , respectively, do not enter the influence action in eq. (4.32), a more detailed explanation can be found in [8]. Hence we obtain

$$S_{\text{infl}} = \frac{\eta}{4\pi} \int d\tau \int d\tau' \frac{(q(\tau) - q(\tau'))^2}{(\tau - \tau')^2}. \quad (4.34)$$

The influence action was derived for linear and non-local coupling, ohmic dissipation and zero temperature. Except for the non-local coupling the microscopic system fulfills all these conditions. Therefore the difference in the coupling will lead to a different influence action. The effective action for the system coupled to the environment reads

$$S_{\text{eff}} = S_S + S_{\text{infl}} = \int d\tau \left(\frac{1}{2} M \dot{q}^2 + V(q) \right) + \frac{\eta}{4\pi} \int d\tau \int d\tau' \frac{(q(\tau) - q(\tau'))^2}{(\tau - \tau')^2}. \quad (4.35)$$

4.2 Effective action in the TB model

The formulation of the effective action in the TB model leads to the Coulomb gas formulation of the influence action, which provides a suitable framework to elaborate the difference between the microscopic system and the spin-boson or Caldeira Leggett system.

4.2.1 Influence action in the charge picture

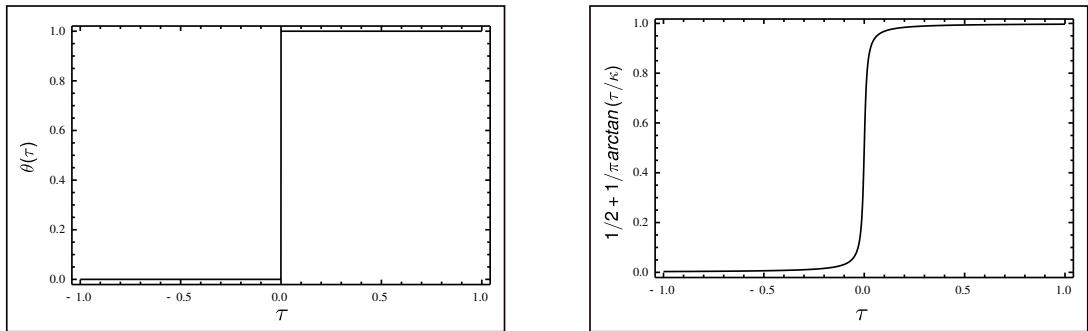


Figure 4.1 Left panel shows the step function and the right panel the analytic approximation by the arctan-function for $\kappa = 0.01$.

We follow the calculation presented in [5]. In the TB ansatz the path of the particle can be expressed in terms of charges e_i

$$q(\tau) = q_0 \sum_i e_i \theta(\tau - \tau_i) \stackrel{\tau_i \text{ arbitrary}}{=} q_0 \sum_i e_i f(\tau - \tau_i). \quad (4.36)$$

We can now use the continuous Fourier transformation and derive eq. (4.36) with respect to τ

$$\begin{aligned} \int d\tau \partial_\tau q(\tau) e^{-i\omega\tau} &= q_0 \int d\tau \partial_\tau \sum_i e_i f(\tau) e^{-i\omega(\tau - \tau_i)} \\ -i\omega \underbrace{\int d\tau q(\tau) e^{-i\omega\tau}}_{q(\omega)} &= q_0 \underbrace{\int d\tau \partial_\tau f(\tau) e^{-i\omega\tau}}_{h(\omega)} \sum_i e_i e^{i\omega\tau_i} \\ \Rightarrow q(\omega) &= q_0 \frac{i}{\omega} h(\omega) \sum_i e_i e^{i\omega\tau_i}. \end{aligned} \quad (4.37)$$

In order to calculate the Fourier transformed coordinate $q(\omega)$ of the particle, we analytically approximate the step function

$$\theta(\tau) = \frac{1}{2} + \lim_{\kappa \rightarrow 0} \frac{1}{\pi} \arctan\left(\frac{\tau}{\kappa}\right). \quad (4.38)$$

The parameter κ defines the width of the jump. The smaller the parameter κ , the greater is the steepness, or expressed in time, the faster is the tunneling process. Hence the step function describes an instantaneous tunneling process and the *arctan*-function describes the tunneling process that costs a certain amount of time $\Delta\tau$. The functions are compared in Figure 4.1. The constant term $1/2$ in eq. (4.38) has no relevance, because it would lead to a constant term in the action, which has no impact on the physics. We therefore make the following TB ansatz

$$f(\tau) = \frac{1}{\pi} \arctan\left(\frac{\tau}{\kappa}\right). \quad (4.39)$$

Derivation with respect to τ yields

$$\partial_\tau f(\tau) = \frac{1}{\pi} \frac{\kappa}{\tau^2 + \kappa^2}. \quad (4.40)$$

This expression can be Fourier transformed

$$h(\omega) = \frac{1}{\pi} \int d\tau \frac{\kappa}{\tau^2 + \kappa^2} e^{-i\omega\tau} = e^{-\kappa|\omega|}. \quad (4.41)$$

The results of Eq. (4.40) and Eq. (4.41) can be found in [15] Tab. 8.1 and 21.14.3. Inserting eq. (4.41) into eq. (4.37) and assuming that $\omega \in \mathbb{R}$, we obtain

$$\begin{aligned} q(\omega) &= q_0 \frac{i}{\omega} e^{-\kappa|\omega|} \sum_i e_i e^{i\omega\tau_i}, \\ q^*(\omega) &= -q_0 \frac{i}{\omega} e^{-\kappa|\omega|} \sum_i e_i e^{-i\omega\tau_i}. \end{aligned} \quad (4.42)$$

With the above relations the influence action in momentum space of eq. (4.28) reads

$$\begin{aligned}
S_{\text{infl}} &= \frac{\eta}{4\pi} \int d\omega |\omega| q(\omega) q^*(\omega) \\
&= \frac{q_0^2 \eta}{4\pi} \int_{-\infty}^{\infty} d\omega |\omega| \left(\frac{i}{\omega} e^{-\kappa|\omega|} \sum_i e_i e^{i\omega\tau_i} \right) \left(-\frac{i}{\omega} e^{-\kappa|\omega|} \sum_j e_j e^{-i\omega\tau_j} \right) \\
&= \frac{q_0^2 \eta}{4\pi} \sum_{i,j} e_i e_j \int_{-\infty}^{\infty} d\omega \frac{1}{|\omega|} e^{-2\kappa|\omega|} e^{i\omega(\tau_i - \tau_j)}
\end{aligned} \tag{4.43}$$

We use the relation between the charges of eq. (4.85)

$$\sum_{i \neq j}^n e_i e_j = \sum_{i,j}^n e_i e_j - \sum_i^n e_i^2 \quad \Rightarrow \quad \sum_{i,j}^n e_i e_j = \sum_{i \neq j}^n e_i e_j + \sum_i^n e_i^2. \tag{4.44}$$

Then the influence action of eq. (4.43) reads

$$\begin{aligned}
S_{\text{infl}} &= \frac{q_0^2 \eta}{4\pi} \left(\sum_{i \neq j}^n e_i e_j + \sum_i^n e_i^2 \right) \int_{-\infty}^{\infty} d\omega \frac{1}{|\omega|} e^{-2\kappa|\omega|} e^{i\omega(\tau_i - \tau_j)} \\
&= \frac{q_0^2 \eta}{4\pi} \left[\sum_{i \neq j}^n e_i e_j \int_{-\infty}^{\infty} d\omega \frac{1}{|\omega|} e^{-2\kappa|\omega|} e^{i\omega(\tau_i - \tau_j)} + \sum_i^n e_i^2 \int_{-\infty}^{\infty} d\omega \frac{1}{|\omega|} e^{-2\kappa|\omega|} \underbrace{e^{i\omega(\tau_i - \tau_i)}}_{=1} \right].
\end{aligned} \tag{4.45}$$

Since we consider charges $e_i = \pm 1$, we can replace

$$\sum_i^n e_i^2 = \sum_i^n 1 = n, \tag{4.46}$$

and obtain for the influence action

$$S_{\text{infl}} = \frac{q_0^2 \eta}{4\pi} \left[\sum_{i \neq j}^n e_i e_j \int_{-\infty}^{\infty} d\omega \frac{1}{|\omega|} e^{-2\kappa|\omega|} e^{i\omega(\tau_i - \tau_j)} + n \int_{-\infty}^{\infty} d\omega \frac{1}{|\omega|} e^{-2\kappa|\omega|} \right]. \tag{4.47}$$

We can use the result of eq. (4.88), that was obtain by implementing the neutrality condition

$$\sum_{i \neq j}^n e_i e_j = -n \quad \Rightarrow \quad n = - \sum_{i \neq j}^n e_i e_j. \tag{4.48}$$

Then the influence action becomes

$$\begin{aligned}
S_{\text{infl}} &= \frac{q_0^2 \eta}{4\pi} \left[\sum_{i \neq j}^n e_i e_j \int_{-\infty}^{\infty} d\omega \frac{1}{|\omega|} e^{-2\kappa|\omega|} e^{i\omega(\tau_i - \tau_j)} - \sum_{i \neq j}^n e_i e_j \int_{-\infty}^{\infty} d\omega \frac{1}{|\omega|} e^{-2\kappa|\omega|} \right] \\
&= \frac{q_0^2 \eta}{4\pi} \sum_{i \neq j}^n e_i e_j \int_{-\infty}^{\infty} d\omega \frac{1}{|\omega|} e^{-2\kappa|\omega|} \left[e^{i\omega(\tau_i - \tau_j)} - 1 \right] \\
&= -\frac{q_0^2 \eta}{4\pi} \sum_{i \neq j}^n e_i e_j \log \left(\frac{\kappa^2 + (\tau_i - \tau_j)^2/4}{\kappa^2} \right).
\end{aligned} \tag{4.49}$$

As mentioned above the tunneling process itself can be assumed to be nearly instantaneous, hence the parameter κ is very small. Also the quantum mechanical probability for the tunneling process between two neighboring minima is very small. Taking these considerations into account, we conclude

$$\kappa \ll \tau_i - \tau_j. \quad (4.50)$$

In this case the influence action of eq. (4.49) can be written as

$$\begin{aligned} S_{\text{infl}} &= -\frac{q_0^2 \eta}{4\pi} \sum_{i \neq j}^n e_i e_j \log \left(\frac{(\tau_i - \tau_j)^2}{4\kappa^2} \right) \\ &= -\frac{q_0^2 \eta}{4\pi} \sum_{i \neq j}^n e_i e_j 2 \log \left(\frac{|\tau_i - \tau_j|}{2\kappa} \right) \\ &= -\frac{q_0^2 \eta}{2\pi} \sum_{i \neq j}^n e_i e_j \log \left(\frac{|\tau_i - \tau_j|}{2\kappa} \right) = -\frac{q_0^2 \eta}{2\pi} \sum_{i \neq j}^n e_i e_j \log \left(\frac{|\tau_i - \tau_j|}{\tau} \right), \end{aligned} \quad (4.51)$$

where we chose the cut-off or minimum kink/antikink separation to be $2\kappa = \tau$. In the charge representation of the influence action the coupling between the environment and the particle is expressed as a logarithmic interaction between the charges. This model is also named Coulomb gas model, so in the case of a equal number of positive and negative charges one speaks of a neutral gas. The indices i and j are different, so self interactions are excluded. The effective action in the TB model reads

$$\begin{aligned} S_{\text{eff}}^{\text{TB}} &= S_S + S_{\text{infl}} \\ &= ns - \frac{q_0^2 \eta}{2\pi} \sum_{i,j}^n e_i e_j \log \frac{|\tau_i - \tau_j|}{\tau}, \end{aligned} \quad (4.52)$$

where s is the action of a single kink/antikink, for a path of n kinks and antikinks it appears n times.

4.3 Interaction Lagrangian and influence action for the microscopic system

To form the influence action for our system, we revisit the result of eq. (4.34) for the Caldeira Leggett model that has been derived for linear coupling

$$S_{\text{infl}} = \frac{\eta}{4\pi} \int d\tau \int d\tau' \frac{(q(\tau) - q(\tau'))^2}{(\tau - \tau')^2}. \quad (4.53)$$

The influence action is non-local and does not depend on the position of the particle. In our system the minima of the potential are overlaid with bose tubes. Therefore the particle can only couple to one of the bose tubes if it is in one of the minima x_j of the potential. This constraint can be formally expressed by replacing the coordinate $q(\tau)$ of the particle by a delta function

$$q(\tau) \rightarrow q_0 \sum_j \delta(q(\tau) - x_j). \quad (4.54)$$

For every well the delta function evaluates whether the particle is in the minimum of the well or not

$$\delta(q(\tau) - k_j) = \begin{cases} 0 & \text{if } q(\tau) \neq x_j \\ 1 & \text{if } q(\tau) = x_j \end{cases}. \quad (4.55)$$

In this sense the path of the particle through the potential is split into j paths for every single well. Consequently the coordinate of the particle in the interaction term of the Euclidean Lagrangian in eq. (2.52) has to be replaced according to eq. (4.54)

$$L_I = - \sum_{\alpha} c_{\alpha} x_{\alpha} q \rightarrow L_I^{\delta} = - \sum_{\alpha, j} c_{\alpha} x_{\alpha}^j q_0 \delta(q - x_j), \quad (4.56)$$

so the particle couples to the coordinates x_{α}^j of the j 'th bose tube if it is in the x_j 'th minimum. As the coupling is still linear the form of the interaction term has not changed, hence the derivation of the influence action in section (4.1.1) does not change except for the replacement of the coordinate q

$$S_{\text{infl}}^{\delta} = \frac{\eta}{4\pi} \sum_j \int d\tau \int d\tau' \frac{(q_0 \delta(q(\tau) - k_j) - q_0 \delta(q(\tau') - k_j))^2}{(\tau - \tau')^2}. \quad (4.57)$$

The system is no longer called 'microscopic system', but will now be called δ -system due to the form of the interaction.

4.3.1 Double well and delta double well

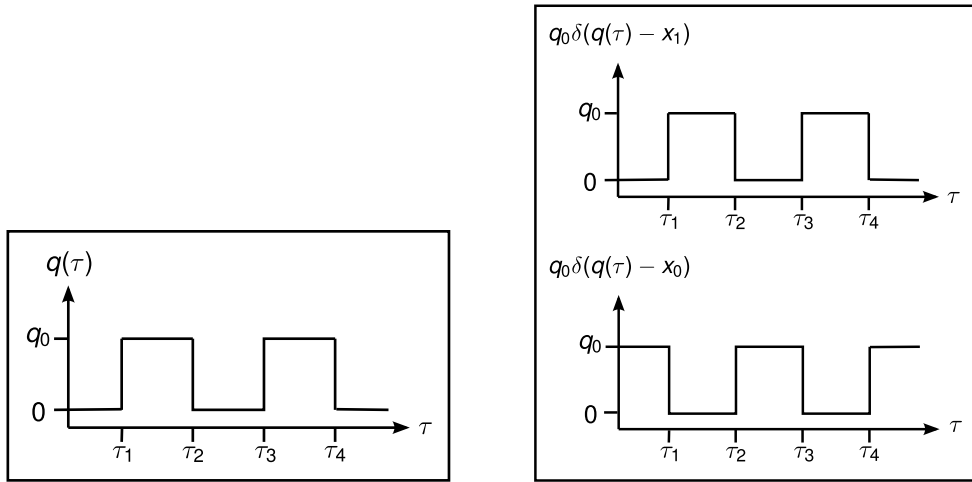


Figure 4.2 The right panel shows the path of a particle in the double well, with an alternating sequence of kinks and antikinks. The right panel shows the paths of each well, which are complementary.

In order to study the difference between the delta system and the Caldeira Leggett system with continuous coupling, we have to find a relation between the path through the potential and the

path for each well as it is motivated in eq. (4.54). For a start we are going to have a look at the double well. The two minima of the potential with minimum separation q_0 are chosen to be

$$x_0 = 0 \quad \text{and} \quad x_1 = q_0. \quad (4.58)$$

In the TB model the particle in a double well has two possible positions

$$q(\tau) = x_0 = 0 \quad \text{and} \quad q(\tau) = x_1 = q_0, \quad (4.59)$$

so it will tunnel back and forth in the double well between the two minima. In this case the relation between the path $q(\tau)$ through the potential and the paths for each well is quite simple, because the particle has only two options. Strictly speaking, we know that the particle has to be in the well x_0 , if it is not in the well x_1

$$\begin{aligned} q_0 \delta(q(\tau) - x_0) &= q_0 - q(\tau) = \begin{cases} 0, & \text{if } q(\tau) = q_0 \\ q_0, & \text{if } q(\tau) = 0 \end{cases}, \\ q_0 \delta(q(\tau) - x_1) &= q(\tau) = \begin{cases} q_0, & \text{if } q(\tau) = q_0 \\ 0, & \text{if } q(\tau) = 0 \end{cases}. \end{aligned} \quad (4.60)$$

The path for every single well evaluates at which time the particle comes into the well and at which time it leaves the well. The comparison of the paths is shown in Figure 4.2. Inserting the relations of eq. (4.60) yields the influence action for the delta double well

$$\begin{aligned} S_{\text{infl}}^{\delta\text{-double}} &= \frac{\eta}{4\pi} \sum_{j=0}^1 \int d\tau \int d\tau' \frac{(q_0 \delta(q(\tau) - x_j) - q_0 \delta(q(\tau') - x_j))^2}{(\tau - \tau')^2} \\ &= \frac{\eta}{4\pi} \left(\int d\tau \int d\tau' \frac{(q_0 \delta(q(\tau) - x_0) - q_0 \delta(q(\tau') - x_0))^2}{(\tau - \tau')^2} \right. \\ &\quad \left. + \int d\tau \int d\tau' \frac{(q_0 \delta(q(\tau) - x_1) - q_0 \delta(q(\tau') - x_1))^2}{(\tau - \tau')^2} \right) \end{aligned} \quad (4.61)$$

Inserting eq. (4.60) into eq. (4.61) we obtain

$$S_{\text{infl}}^{\delta\text{-double}} = \frac{\eta}{4\pi} \left(\int d\tau \int d\tau' \frac{(q_0 - q(\tau) - (q_0 - q(\tau')))^2}{(\tau - \tau')^2} + \int d\tau \int d\tau' \frac{(q(\tau) - q(\tau'))^2}{(\tau - \tau')^2} \right) \quad (4.62)$$

$$= \frac{\eta}{4\pi} \left(\int d\tau \int d\tau' \frac{(q(\tau') - q(\tau))^2}{(\tau - \tau')^2} + \int d\tau \int d\tau' \frac{(q(\tau) - q(\tau'))^2}{(\tau - \tau')^2} \right) \quad (4.63)$$

$$= 2 \frac{\eta}{4\pi} \int d\tau \int d\tau' \frac{(q(\tau) - q(\tau'))^2}{(\tau - \tau')^2} \quad (4.64)$$

Since the coordinate $q(\tau)$ is describing the motion of a particle in a double well without the constraints of two bose tubes, we can conclude

$$S_{\text{infl}}^{\delta\text{-double}} = 2 S_{\text{infl}}^{\text{double}} \quad (4.65)$$

4.4 Influence action for the delta system in the charge picture

The coupling between the environment and the particle in the charge picture is expressed as interactions between the charges. Therefore a change in the coupling manifests itself in a change of the interactions. For the interactions in the case of continuous coupling there are only two restrictions. The total number of charges has to be zero and there are no self interactions, apart from the fact that every charge e_i interacts with every other charge e_j

$$S_{\text{infl}} = -\frac{\eta q_0^2}{2\pi} \sum_{i \neq j} e_i e_j \log \frac{|\tau_i - \tau_j|}{\tau}. \quad (4.66)$$

This can no longer be true for the delta system, because the coupling is restricted to each well. Accordingly, only the charges or kinks and antikinks belonging to one well interact with each other. To find an exact expression for the interactions in the case of the delta lattice we have to determine for an arbitrary path when the particle is in which well. For the description in the charge picture, we will use the same notation and assumptions as introduced in section 2.7. So the initial charge is e_1 at τ_1 with $e_0 \stackrel{!}{=} 0$, the necessity of this choice will become clear later on.

4.4.1 Charge condition

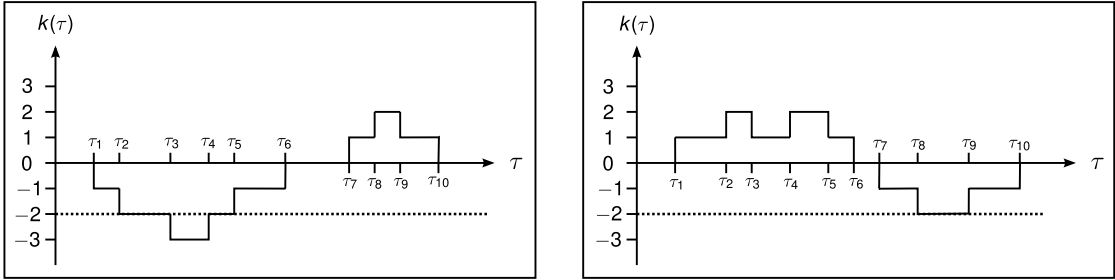


Figure 4.3 Two exemplary TB paths in a lattice.

To solve the problem we can adopt the idea of the delta function in eq. (4.54) and rewrite it as a charge condition

$$\delta \left(\sum_{l=0}^j e_l - k \right) = \begin{cases} 1, & \text{if } \sum_{l=0}^j e_l = k \rightarrow \text{particle is in well } k \\ 0, & \text{if } \sum_{l=0}^j e_l \neq k \rightarrow \text{particle is not in well } k \end{cases}. \quad (4.67)$$

The delta function is based on the fact, that the sum over all charges from e_1 at τ_1 to the charge e_j at τ_j has to be 0 in order to be in the well $k = 0$ at τ_j and has to be 1 in order to be in the well $k = 1$ at τ_j and so on. This condition is path-independent as shown for two paths in Figure 4.3. The dashed line shows the $k = -2$ -well. For the left path the particle reaches the well at τ_2 and τ_4 , we can read off the distribution of the charges and hence the sum of the charges yields

$$e_1 + e_2 = -1 - 1 = -2, \quad e_1 + e_2 + e_3 + e_4 = -1 - 1 - 1 + 1 = -2. \quad (4.68)$$

For the right path in Figure 4.3 the particle reaches the $k = -2$ -well at τ_8 . In this case the sum of the charges is

$$e_1 + e_2 + e_3 + e_4 + e_5 + e_6 + e_7 + e_8 = +1 + 1 - 1 + 1 - 1 - 1 - 1 - 1 = -2. \quad (4.69)$$

4.4.2 Interactions for the path of each well

Since we are interested in the interactions between the kinks and antikinks belonging to one well, we have to think about the general structure for the path of each well. In section 4.3.1 we discussed how the path through the delta double well is split into two paths, which in principle does not change for the delta lattice. The path of each well has the structure

$$\dots - \text{kink} - \text{antikink} - \text{kink} - \text{antikink} - \dots \quad \text{or} \quad \dots + - + - \dots \quad . \quad (4.70)$$

There are three possible interactions for each path

$$\begin{aligned} \text{kink} &\leftrightarrow \text{kink} = (\text{KK}) \\ \text{kink} &\leftrightarrow \text{antikink} = (\text{KA}) \\ \text{antikink} &\leftrightarrow \text{antikink} = (\text{AA}) \quad . \end{aligned} \quad (4.71)$$

We now have to express these cases in terms of the charge condition in eq. (4.67). The kink appears because the particle comes into the well and the antikink because it leaves the well. The kink satisfies the charge condition, whereas the antikink appears because the kink before satisfied the charge condition. To express the appearance of the antikink we therefore have to shift the index j in the charge condition

$$\delta \left(\sum_{l=0}^{i-1} e_l - k \right). \quad (4.72)$$

One has to understand that we could not have shifted the k value, because the interactions have to belong to the same well. Since not only neighboring kinks and antikinks interact with each other, we have introduced a second index i that runs independently from j . In the case of an KA-interaction both conditions in eq. (4.67) and (4.72) have to be fulfilled, so that the interaction condition is built as a product of delta functions. The same arguments hold for the KK- and AA-interaction

$$\begin{aligned} \text{KK} &\rightarrow \sum_{i \neq j} \delta \left(\sum_l^j e_l - k \right) \delta \left(\sum_l^i e_l - k \right), \\ \text{KA} &\rightarrow \sum_{i \neq j} \delta \left(\sum_l^j e_l - k \right) \delta \left(\sum_l^{i-1} e_l - k \right), \\ \text{AA} &\rightarrow \sum_{i \neq j} \delta \left(\sum_l^{j-1} e_l - k \right) \delta \left(\sum_l^{i-1} e_l - k \right), \end{aligned} \quad (4.73)$$

where the well k is arbitrary, but determined. As self interactions are not allowed the indices i and j have to be different. The interaction between all the kinks/antikinks for one well can be physically interpreted as a memory of each bose tube.

4.4.3 Exact expression for the influence action of the delta-system

With the considerations of the previous section we are able to give the exact influence action for the delta system

$$\begin{aligned}
S_{\text{infl}}^{\delta} &= -\frac{q_0^2 \eta}{2\pi} \sum_{k=0}^K \sum_{i \neq j}^n (-1)^{|i-j|} \left[\delta \left(\sum_l^j e_l - k \right) + \delta \left(\sum_l^{j-1} e_l - k \right) \right] \times \\
&\quad \times \left[\delta \left(\sum_l^i e_l - k \right) + \delta \left(\sum_l^{i-1} e_l - k \right) \right] \log |\tau_i - \tau_j| \\
&\stackrel{(*)}{=} -\frac{q_0^2 \eta}{2\pi} \sum_{k=0}^K \sum_{i \neq j}^n \underbrace{\left[\delta \left(\sum_l^j e_l - k \right) \delta \left(\sum_l^i e_l - k \right) \right]}_{\text{KK}} \\
&\quad - \underbrace{\left[\delta \left(\sum_l^j e_l - k \right) \delta \left(\sum_l^{i-1} e_l - k \right) - \delta \left(\sum_l^{j-1} e_l - k \right) \delta \left(\sum_l^i e_l - k \right) \right]}_{\text{KA}} \\
&\quad + \underbrace{\left[\delta \left(\sum_l^{j-1} e_l - k \right) \delta \left(\sum_l^{i-1} e_l - k \right) \right]}_{\text{KK}} \log |\tau_i - \tau_j|. \tag{4.74}
\end{aligned}$$

In the general case we have to sum over all K wells and all n kinks and antikinks. The expression is symmetric in the indices i and j . In $(*)$ we made use of the fact that the sign of the interaction term is determined for the three cases

$$(KK) = (++) = \oplus, \quad (KA) = (+-) = \ominus, \quad (AA) = (--) = \oplus. \tag{4.76}$$

The alternative determination of the sign in eq. (4.74) is based on the fact that the path for each well has the same structure as the double well path. From this we can conclude that the distance in τ between a kink(antikink) at τ_i and a kink(antikink) at τ_j is even, whereas the distance between a kink(τ_i) and a antikink(τ_j) is not even

$$\text{sign} = (-1)^{|i-j|} = \begin{cases} +1 & \text{for KK and AA} \\ -1 & \text{for KA} \end{cases} \tag{4.77}$$

In order to reproduce all interaction terms for the $k = 0$ -well, we have to place a condition on the evaluation of the influence action

$$\sum_{l=0}^0 e_l \stackrel{!}{=} 0 \quad \text{with} \quad e_0 = 0. \tag{4.78}$$

This can be understood, considering the appearance of the first antikink at τ_1 for $k = 0$. The antikink occurs because the charge condition was satisfied before it. Since there is no kink before τ_1 , the interactions between τ_1 and the other kinks and antikinks for $k = 0$ could not be reproduced from eq. (4.75) without the condition of eq. (4.78). Clearly it does not affect the results for the wells with $k > 0$, because $\delta(0 - (k > 0))$ is always zero.

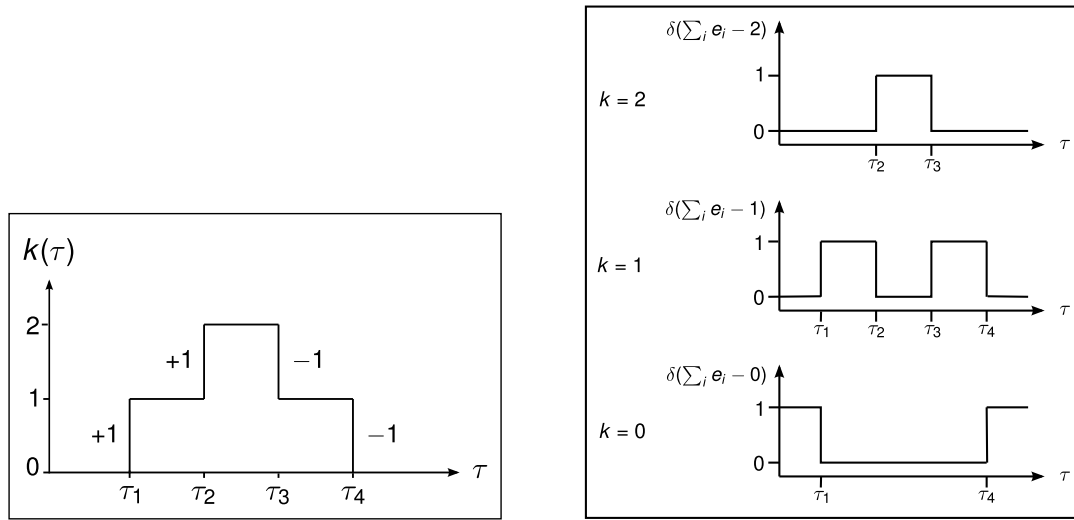


Figure 4.4 The left panel shows four steps of a TB path in three wells. The left panel shows the paths of each well.

Example

In order to give an understanding how the formula works, we will consider a concrete path with four moves in three wells. We are going to write out the evaluation of the KK-interaction for the well $k = 1$. According to the formula in eq. (4.75) the (KK)-interactions for $k = 1$ with $n = 4$ are given by

$$\begin{aligned}
& \sum_{i \neq j}^4 \delta \left(\sum_{l=0}^j e_l - 1 \right) \delta \left(\sum_{l=0}^i e_l - 1 \right) \log |\tau_j - \tau_i| \\
&= \delta \left(\sum_{l=0}^1 e_l - 1 \right) \delta \left(\sum_{l=0}^2 e_l - 1 \right) \log |\tau_1 - \tau_2| + \delta \left(\sum_{l=0}^2 e_l - 1 \right) \delta \left(\sum_{l=0}^1 e_l - 1 \right) \log |\tau_2 - \tau_1| \\
&+ \delta \left(\sum_{l=0}^1 e_l - 1 \right) \delta \left(\sum_{l=0}^3 e_l - 1 \right) \log |\tau_1 - \tau_3| + \delta \left(\sum_{l=0}^3 e_l - 1 \right) \delta \left(\sum_{l=0}^1 e_l - 1 \right) \log |\tau_3 - \tau_1| \\
&+ \delta \left(\sum_{l=0}^1 e_l - 1 \right) \delta \left(\sum_{l=0}^4 e_l - 1 \right) \log |\tau_1 - \tau_4| + \delta \left(\sum_{l=0}^4 e_l - 1 \right) \delta \left(\sum_{l=0}^1 e_l - 1 \right) \log |\tau_4 - \tau_1| \\
&+ \delta \left(\sum_{l=0}^2 e_l - 1 \right) \delta \left(\sum_{l=0}^3 e_l - 1 \right) \log |\tau_2 - \tau_3| + \delta \left(\sum_{l=0}^3 e_l - 1 \right) \delta \left(\sum_{l=0}^2 e_l - 1 \right) \log |\tau_3 - \tau_2| \\
&+ \delta \left(\sum_{l=0}^2 e_l - 1 \right) \delta \left(\sum_{l=0}^4 e_l - 1 \right) \log |\tau_2 - \tau_4| + \delta \left(\sum_{l=0}^4 e_l - 1 \right) \delta \left(\sum_{l=0}^2 e_l - 1 \right) \log |\tau_4 - \tau_2| \\
&+ \delta \left(\sum_{l=0}^3 e_l - 1 \right) \delta \left(\sum_{l=0}^4 e_l - 1 \right) \log |\tau_3 - \tau_4| + \delta \left(\sum_{l=0}^4 e_l - 1 \right) \delta \left(\sum_{l=0}^3 e_l - 1 \right) \log |\tau_4 - \tau_3| \\
&= \log |\tau_1 - \tau_3| + \log |\tau_3 - \tau_1|, \tag{4.79}
\end{aligned}$$

where we have evaluated the charge conditions for the particular path with

$$e_1 = +1, \quad e_2 = +1, \quad e_3 = -1, \quad e_4 = -1. \quad (4.80)$$

$$\begin{aligned} \tau_1 < \tau : \quad \sum_{l=0}^0 e_l = 0, & \quad \tau_1 \leq \tau < \tau_2 : \quad \sum_{l=0}^1 e_l = 1 \\ \tau_2 \leq \tau < \tau_3 : \quad \sum_{l=0}^2 e_l = 2, & \quad \tau_3 \leq \tau < \tau_4 : \quad \sum_{l=0}^3 e_l = 1, \\ \tau_4 \leq \tau : \quad \sum_{l=0}^4 e_l = 0 \end{aligned} \quad (4.81)$$

Since the particle moves into the well $k=1$ at τ_1 and τ_3 the kink-charge-condition in eq. (4.67) is fulfilled twice

$$k = 1 = \begin{cases} \sum_{l=0}^1 e_l = 0 + 1 \\ \sum_{l=0}^3 e_l = 0 + 1 + 1 - 1. \end{cases} \quad (4.82)$$

We can conclude that the kinks at τ_1 and τ_3 interact with each other, which matches the result in eq. (4.79). An overview of the evaluation of all the interactions is given in Table 4.1. The structure of the table reflects the most efficient systematic to evaluate eq. (4.75). For every well k the interaction cases KK, KA and AA are listed separately. One has to check for each case which index j fulfills one of the corresponding charge conditions and then find which of the possible indices $i \neq j$ matches the second charge condition in the product of the delta functions. The indices i and j that do not lead to a vanishing product of the delta functions, make up the logarithmic interaction term (ji).

4.4.4 Simplifying the sum over the interacting charges for the SB-system

In the case of the SB-system every charge interacts with every charge excluding self-interaction, the sum has the simple form

$$\sum_{i \neq j}^n e_i e_j = 2e_1 e_2 + 2e_1 e_3 + \dots + 2e_1 e_n + e_2 e_3 + \dots + 2e_2 e_n + \dots + 2e_{n-1} e_n. \quad (4.83)$$

The sum over all combinations, including self-interactions, reads

$$\begin{aligned} \sum_{i,j}^n e_i e_j &= e_1^2 + e_2^2 + \dots + e_n^2 + 2e_1 e_2 + 2e_1 e_3 + \dots + 2e_1 e_n + 2e_2 e_3 + \dots \\ &\dots + 2e_2 e_n + \dots + 2e_{n-1} e_n. \end{aligned} \quad (4.84)$$

The difference between the two sums are the self-interaction terms, therefore we can write

$$\sum_{i \neq j}^n e_i e_j = \sum_{i,j}^n e_i e_j - \sum_i^n e_i^2. \quad (4.85)$$

Using the fact that

$$\begin{aligned} \left(\sum_i^n e_i \right)^2 &= e_1^2 + e_2^2 + \dots + e_n^2 + 2e_1 e_2 + 2e_1 e_3 + \dots \\ &\dots + 2e_1 e_n + 2e_2 e_3 + \dots + 2e_2 e_n + \dots + 2e_{n-1} e_n, \end{aligned} \quad (4.86)$$

well	case	index j	index i	interaction (ji)	sign
$k = 0$	KK	—	—	—	
	KA	4	1, 2, 3	(41)	—
		1	3, 2, 4	(14)	—
	AA	—	—	—	
$k = 1$	KK	1	2, 3, 4	(13)	+
		3	1, 2, 4	(31)	+
	KA	1	2, 3, 4	(12), (14)	—, —
		3	1, 2, 4	(32), (34)	—, —
		2	1, 3, 4	(21), (23)	—, —
		4	1, 2, 3	(41), (43)	—, —
	AA	2	1, 3, 4	(24)	+
4		1, 2, 3	(42)	+	
$k = 2$	KK	—	—	—	
	KA	2	1, 3, 4	(2, 3)	—
		3	1, 2, 4	(3, 2)	—
	AA	—	—	—	

Table 4.1 Overview of the interactions for the exemplary path, listed for each well and case separately.

we can rewrite eq. (4.83) and obtain

$$\sum_{i \neq j}^n e_i e_j = \left(\sum_i^n e_i \right)^2 - \sum_i^n e_i^2. \quad (4.87)$$

The neutrality condition requires the number of positive and negative charges to be equal and therefore the sum over all charges equals zero. Since we consider charges $e_i = \pm 1$, the value of a squared charge is always one

$$\sum_{i \neq j}^n e_i e_j = \underbrace{\left(\sum_i^n e_i \right)^2}_{=0} - \sum_i^n \underbrace{e_i^2}_{=1} = - \sum_i^n 1 = -n. \quad (4.88)$$

We did not choose a specific charge distribution, hence the result is path independent.

4.4.5 Simplifying the sum over the interacting charges for the delta-system

The interactions between the charges for the delta-system are given by

$$\begin{aligned} & \sum_{k=0}^K \sum_{i \neq j}^n \left[\underbrace{\delta \left(\sum_l^j e_l - k \right) \delta \left(\sum_l^i e_l - k \right)}_{\text{KK}} - \right. \\ & \quad \left. - \underbrace{\delta \left(\sum_l^j e_l - k \right) \delta \left(\sum_l^{i-1} e_l - k \right) - \delta \left(\sum_l^{j-1} e_l - k \right) \delta \left(\sum_l^i e_l - k \right)}_{\text{KA}} + \right. \\ & \quad \left. + \underbrace{\delta \left(\sum_l^{j-1} e_l - k \right) \delta \left(\sum_l^{i-1} e_l - k \right)}_{\text{KK}} \right]. \quad (4.89) \end{aligned}$$

We want to determine how many positive and negative interactions occur for an arbitrary path of the particle. Therefore we have to solve the structure of the interactions. For this purpose we can rewrite the above expression as

$$\sum_{k=0}^K \sum_{i \neq j}^n \left[\underbrace{\delta \delta}_{\text{KK}} - \underbrace{\delta \delta}_{\text{KA}} - \underbrace{\delta \delta}_{\text{AK}} + \underbrace{\delta \delta}_{\text{AA}} \right]. \quad (4.90)$$

The neutrality condition requires that the maximal number of wells that the particle can move, is half the number of steps n

$$K = \frac{n}{2}. \quad (4.91)$$

The particle can move at most $n/2$ steps in one direction in a row, because it has to reach the initial well after n steps again. Evaluating the sum over (i, j) in eq. (4.90) yields for every summand k the terms

$$n(n-1)[\text{KK}] - n(n-1)[\text{KA}] - n(n-1)[\text{AK}] + n(n-1)[\text{AA}]. \quad (4.92)$$

One has to remember that not all of these possible terms for each well k fulfill the charge condition, like shown for an exemplary path in Table 4.1. Examples suggest that the evaluation of the sum over all k wells yields for the number of positive and negative charge interactions

$$\sum_{k=0}^{n/2} (n(n-1)[KK] - n(n-1)[KA] - n(n-1)[AK] + n(n-1)[AA]) = -2n. \quad (4.93)$$

The above result differs from the result of eq. (4.88) for the SB-system. In the case of the double well the factor 2 can be graphically understood by regarding Figure 4.2. The path splits up into the identical path and the complementary path with the same number of kinks and antikinks. Therefore the number of the interactions is doubled. Since the structure is identical the number of additional positive and negative signs is equal and thus leads to a factor of 2. In the more general example in Figure 4.4 the relation between the SB-system and the delta-system is not as apparent as for the double well. Clearly the distribution of the additional interactions on the particular wells is path-dependent, nonetheless the sum over all the signs of the interactions is doubled for an arbitrary path. In Table 4.1 the signs of the interactions for $n = 4$ steps are listed in the last column, the sum yields

$$12 \times (-) + 4 \times (+) = -8 = -2n. \quad (4.94)$$

For the general path in the left panel of Figure 4.4 the interactions and the corresponding signs read

$$\begin{aligned} KK : (12), (21) &\rightarrow 2 \times (+) \\ KA : (13), (31) &\rightarrow 2 \times (-) \\ &(14), (41) \rightarrow 2 \times (-) \\ &(23), (32) \rightarrow 2 \times (-) \\ &(24), (42) \rightarrow 2 \times (-) \\ AA : (34), (43) &\rightarrow 2 \times (+). \end{aligned} \quad (4.95)$$

All together the sum over the signs of the interactions for $n = 4$ steps yields

$$8 \times (-) + 4 \times (+) = -4 = -n. \quad (4.96)$$

In the special case of the double well the factor of 2 has been already derived in eq. (4.65) and is now confirmed in the charge picture for an arbitrary path.

Quantum phase transition

5.1 Renormalization group and quantum phase transition

A phase transition at zero temperature can not be described in the framework of classical phase transitions, since there are no thermal fluctuations present. One must conclude that the phase transition occurs due to quantum fluctuations, therefore it is called a quantum phase transition. In analogy to the classical case one speaks of first order and second order quantum phase transitions. The continuous second order phase transition is determined by a quantum critical point, where the intrinsic length scale of the system, also called correlation length ξ , diverges. Hence the system at the quantum critical point is scale-invariant. This is why the theory of second order quantum phase transitions is linked to the renormalization group (RG) method. The basic idea of the RG is to gain information about the system by increasing the length scale and checking how the parameters of the system change under the renormalization. For further reading see [10, 16, 17].

5.2 Partition function in the TB model

The path integral formulation of the partition function was derived in section 2.4. We then introduced the partition function for the 'system plus environment' Lagrangian and arrived at the reduced partition function with effective action

$$Z = \int \mathcal{D}[q(\tau)] e^{-\frac{1}{\hbar} S_{\text{eff}}(q(\tau))}, \quad (5.1)$$

where the coordinates of the environment have been integrated out. The path integral includes all reasonable smooth paths for the propagation of a particle between two points. In the TB limit this description is not appropriate any more, since the evolution of the particle is restricted to the kink/antikink path. Consequently the functional integral has to be replaced by an integration over n kinks and antikinks

$$Z = \sum_n \frac{1}{n!} \int \frac{d\tau_n}{\tau} \dots \int \frac{d\tau_1}{\tau} e^{-\frac{1}{\hbar} S_{\text{eff}}^{\text{TB}}(n)}, \quad (5.2)$$

where the effective action is expressed in the TB formulation, indicated by the superscript TB. Since the partition function is a dimensionless quantity the measure has been divided by τ , which is the minimal distance between two neighboring kinks. From statistics we know that there are $n!$ possibilities to arrange n kinks. Since all these arrangements do not differ in their physical properties they are indistinguishable and we can therefore multiply the expression with a factor $\frac{1}{n!}$.

5.3 Renormalization of the partition function

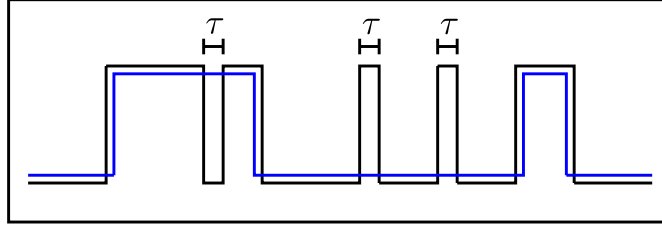


Figure 5.1 The black line draws the problem with minimal kink/antikink separation of τ and the blue line shows the problem after the minimal length scale has been increased to $\tau + d\tau$ (adopted from [7]).

In order to perform the renormalization of the partition function we follow the calculation in [18]. Inserting the influence action of the delta-system in eq. (4.75) into the TB effective action of eq. (4.52) yields

$$S_{\text{eff}}^{\text{TB,delta}} = ns - \frac{q_0^2 \eta}{2\pi} \sum_{k=0}^K \sum_{i \neq j}^n (-1)^{|i-j|} \left[\delta \left(\sum_l^j \mathbf{e}_l - k \right) + \delta \left(\sum_l^{j-1} \mathbf{e}_l - k \right) \right] \times \\ \times \left[\delta \left(\sum_l^i \mathbf{e}_l - k \right) + \delta \left(\sum_l^{i-1} \mathbf{e}_l - k \right) \right] \log |\tau_i - \tau_j|. \quad (5.3)$$

Then the partition function of eq. (5.2) for the delta-system reads

$$Z = \sum_n \frac{1}{n!} \int_{D_n} \frac{d\tau_n}{\tau} \dots \int_{D_1} \frac{d\tau_1}{\tau} \exp \left[-n \frac{s}{\hbar} + \frac{q_0^2 \eta}{2\pi \hbar} \sum_k \sum_{i \neq j}^n (-1)^{|i-j|} \left(\delta \left(\sum_l^j \mathbf{e}_l - k \right) + \delta \left(\sum_l^{j-1} \mathbf{e}_l - k \right) \right) \right] \times \\ \times \left(\delta \left(\sum_l^i \mathbf{e}_l - k \right) + \delta \left(\sum_l^{i-1} \mathbf{e}_l - k \right) \right) \log \left(\frac{|\tau_i - \tau_j|}{\tau} \right) \Big] \\ = \sum_n \frac{1}{n!} \int_{D_n} \frac{d\tau_n}{\tau} \dots \int_{D_1} \frac{d\tau_1}{\tau} \lambda^n \exp \left[\alpha \sum_k \sum_{i \neq j}^n (-1)^{|i-j|} \left(\delta \left(\sum_l^j \mathbf{e}_l - k \right) + \delta \left(\sum_l^{j-1} \mathbf{e}_l - k \right) \right) \right] \times \\ \times \left(\delta \left(\sum_l^i \mathbf{e}_l - k \right) + \delta \left(\sum_l^{i-1} \mathbf{e}_l - k \right) \right) \log \left(\frac{|\tau_i - \tau_j|}{\tau} \right) \Big]. \quad (5.4)$$

In the above equation we inserted the coupling strength α and introduced the parameter

$$\lambda = e^{-\frac{s}{\hbar}}. \quad (5.5)$$

The above partition function has the minimal length scale τ with integration region D_n , hence it takes all kinks/antikinks with separation $\geq \tau$ into account. If we increase the minimal length scale from τ to $\tau' = \tau + d\tau$ with $d\tau \ll \tau$, only kinks/antikinks with separation $\geq \tau + d\tau$ are included, as shown in Figure 5.1. The partition function of the new system can be obtained from the partition function of the initial problem in eq. (5.4) by integrating over all kinks/antikinks with separation $\leq \tau + d\tau$. In our case we do not explicitly perform the integration, but focus on the rescaling. This short cut can be understood by considering the physical meaning of the flow equations and how they are derived in the calculation. The problem depends on the parameters λ , α and the scaling length τ . The renormalization therefore yields two coupled flow equations of the form

$$\begin{aligned} \frac{d\lambda}{dl} &= \beta_\lambda(\lambda, \alpha) \\ \frac{d\alpha}{dl} &= \beta_\alpha(\lambda, \alpha), \end{aligned} \quad (5.6)$$

with $l = \ln \tau$. The first equation can be obtained by performing the rescaling and the second equation comes from the integration over the kinks/antikinks of the initial problem. Since the flow of the parameter λ reveals the critical coupling strength, which is our main interest, it answers our purposes only to do the rescaling. The partition function of the new problem where the integration region is scaled from D_n to D'_n reads

$$\begin{aligned} Z &= \sum_n \frac{1}{n!} \int_{D'_n} \frac{d\tau'_n}{\tau} \dots \int_{D'_1} \frac{d\tau'_1}{\tau} \exp \left[-\frac{S'_{\text{eff}}}{\hbar} \right] \\ &= \sum_n \frac{1}{n!} \int_{D'_n} \frac{d\tau'_n}{\tau} \dots \int_{D'_1} \frac{d\tau'_1}{\tau} \lambda'^n \exp \left[\alpha \sum_k \sum_{i \neq j}^n (-1)^{|i-j|} \left(\delta \left(\sum_l^j e_l - k \right) + \delta \left(\sum_l^{j-1} e_l - k \right) \right) \right. \\ &\quad \left. \times \left(\delta \left(\sum_l^i e_l - k \right) + \delta \left(\sum_l^{i-1} e_l - k \right) \right) \log \left(\frac{|\tau_i - \tau_j|}{\tau} \right) \right]. \end{aligned} \quad (5.7)$$

5.3.1 Rescaling of the partition function describing the new problem

In order to see how the parameters have changed under the scaling, the partition function of eq. (5.7), which describes the new problem, has to be expressed in the initial coordinates τ , which is called rescaling. The integration region transforms like

$$D'_n \rightarrow D_n \quad \text{with} \quad D'_n = D \underbrace{\left(\frac{\tau + d\tau}{\tau} \right)}_{\text{scaling factor}}. \quad (5.8)$$

Accordingly the transformation of the measure reads

$$d\tau' = d\tau \left(\frac{\tau}{\tau + d\tau} \right). \quad (5.9)$$

Performing the transformation by applying the above relation to the partition function of eq. (5.7) yields

$$\begin{aligned}
Z &= \sum_n \frac{1}{n!} \int_{D_n} \frac{d\tau_n}{\tau} \left(\frac{\tau}{\tau + d\tau} \right) \dots \int_{D_1} \frac{d\tau_1}{\tau} \left(\frac{\tau}{\tau + d\tau} \right) \lambda^n \times \\
&\quad \times \exp \left[\alpha \sum_k^K \sum_{i \neq j}^n (-1)^{|i-j|} \left(\delta \left(\sum_l^j \mathbf{e}_l - k \right) + \delta \left(\sum_l^{j-1} \mathbf{e}_l - k \right) \right) \times \right. \\
&\quad \times \left. \left(\delta \left(\sum_l^i \mathbf{e}_l - k \right) + \delta \left(\sum_l^{i-1} \mathbf{e}_l - k \right) \right) \log \left(\frac{|\tau_i - \tau_j|}{\tau} \left(\frac{\tau}{\tau + d\tau} \right) \right) \right] \\
&= \sum_n \frac{1}{n!} \int_{D_n} \frac{d\tau_n}{\tau} \dots \int_{D_1} \frac{d\tau_1}{\tau} \lambda^n \left(\frac{\tau}{\tau + d\tau} \right)^n \times \\
&\quad \times \exp \left[\alpha \sum_k^K \sum_{i \neq j}^n (-1)^{|i-j|} \left(\delta \left(\sum_l^j \mathbf{e}_l - k \right) + \delta \left(\sum_l^{j-1} \mathbf{e}_l - k \right) \right) \times \right. \\
&\quad \times \left. \left(\delta \left(\sum_l^i \mathbf{e}_l - k \right) + \delta \left(\sum_l^{i-1} \mathbf{e}_l - k \right) \right) \left(\log \left(\frac{|\tau_i - \tau_j|}{\tau} \right) + \log \left(\frac{\tau}{\tau + d\tau} \right) \right) \right] \quad (5.10)
\end{aligned}$$

The second summand does not depend on the indices (i, j) , thus the charge interaction term can be replaced by $-2n$, as shown in eq. (4.93). We then obtain

$$\begin{aligned}
Z &= \sum_n \frac{1}{n!} \int_{D_n} \frac{d\tau_n}{\tau} \dots \int_{D_1} \frac{d\tau_1}{\tau} \lambda^n \left(\frac{\tau}{\tau + d\tau} \right)^n \exp \left[\alpha \sum_k^K \sum_{i \neq j}^n (-1)^{|i-j|} \left(\delta \left(\sum_l^j \mathbf{e}_l - k \right) + \delta \left(\sum_l^{j-1} \mathbf{e}_l - k \right) \right) \times \right. \\
&\quad \times \left. \left(\delta \left(\sum_l^i \mathbf{e}_l - k \right) + \delta \left(\sum_l^{i-1} \mathbf{e}_l - k \right) \right) \log \left(\frac{|\tau_i - \tau_j|}{\tau} \right) \right] \underbrace{\exp \left[-2n\alpha \log \left(\frac{\tau}{\tau + d\tau} \right) \right]}_{\left(\frac{\tau}{\tau + d\tau} \right)^{-2n\alpha}} \\
&= \sum_n \frac{1}{n!} \int_{D_n} \frac{d\tau_n}{\tau} \dots \int_{D_1} \frac{d\tau_1}{\tau} \lambda^n \left(\frac{\tau}{\tau + d\tau} \right)^n \left(\frac{\tau}{\tau + d\tau} \right)^{-2n\alpha} \times \\
&\quad \times \exp \left[\alpha \sum_k^K \sum_{i \neq j}^n (-1)^{|i-j|} \left(\delta \left(\sum_l^j \mathbf{e}_l - k \right) + \delta \left(\sum_l^{j-1} \mathbf{e}_l - k \right) \right) \times \right. \\
&\quad \times \left. \left(\delta \left(\sum_l^i \mathbf{e}_l - k \right) + \delta \left(\sum_l^{i-1} \mathbf{e}_l - k \right) \right) \log \left(\frac{|\tau_i - \tau_j|}{\tau} \right) \right] \\
&= \sum_n \frac{1}{n!} \int_{D_n} \frac{d\tau_n}{\tau} \dots \int_{D_1} \frac{d\tau_1}{\tau} \lambda^n \left(\frac{\tau}{\tau + d\tau} \right)^{n(1-2\alpha)} \times \\
&\quad \times \exp \left[\frac{q_0^2 \eta \pi}{\hbar} \sum_k^K \sum_{i \neq j}^n (-1)^{|i-j|} \left(\delta \left(\sum_l^j \mathbf{e}_l - k \right) + \delta \left(\sum_l^{j-1} \mathbf{e}_l - k \right) \right) \times \right. \\
&\quad \times \left. \left(\delta \left(\sum_l^i \mathbf{e}_l - k \right) + \delta \left(\sum_l^{i-1} \mathbf{e}_l - k \right) \right) \log \left(\frac{|\tau_i - \tau_j|}{\tau} \right) \right] \quad (5.11)
\end{aligned}$$

The rescaled partition function describes the new system with increased minimum kink/antikink separation expressed in the initial variable τ with rescaled parameters. It has the same form as the partition function of the initial problem of eq. (5.4). By comparing the above partition function with eq. (5.4) we can see how the parameter λ' changes due to the rescaling

$$\begin{aligned}\lambda'^n &\rightarrow \lambda'^n \left(\frac{\tau}{\tau + d\tau} \right)^{n(1-2\alpha)} = \lambda^n \\ \Rightarrow \lambda'^n &= \lambda^n \left(\frac{\tau + d\tau}{\tau} \right)^{n(1-2\alpha)}\end{aligned}\quad (5.12)$$

5.3.2 Flow equation and critical value

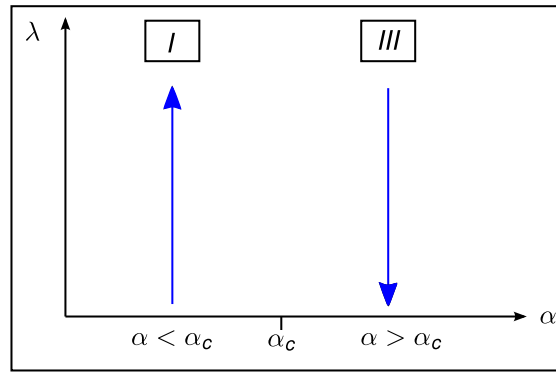


Figure 5.2 The flow of the fugacity changes its sign dependent on the coupling strength. The coupling strength of zero flow can be identified as the critical value α_c .

From the relation between the parameters of the initial and the new problem we can derive the flow equation or Gell-Mann-Low equation. Extracting the root of eq. (5.12) yields

$$\begin{aligned}\lambda' &= \lambda \left(\frac{\tau + d\tau}{\tau} \right)^{(1-2\alpha)} \\ &= \lambda \left(1 + \frac{d\tau}{\tau} \right)^{(1-2\alpha)} \\ &\approx \lambda \left(1 + (1-2\alpha) \frac{d\tau}{\tau} \right) \\ \lambda' &= \lambda + \lambda(1-2\alpha) \frac{d\tau}{\tau}.\end{aligned}\quad (5.13)$$

We can rewrite the last expression to obtain a differential equation for the parameter

$$\frac{\lambda' - \lambda}{d\tau} = \lambda(1-2\alpha) \frac{1}{\tau}.\quad (5.14)$$

It is convenient to substitute the scaling length as follows

$$l = \ln \tau \Rightarrow dl = \frac{d\tau}{\tau}.\quad (5.15)$$

Finally we obtain

$$\frac{d\lambda}{dl} = \lambda(1 - 2\alpha). \quad (5.16)$$

The flow equation tells how the parameter changes if the scaling length τ is changed. We can distinguish between three cases

$$\frac{d\lambda}{dl} \text{ is } \begin{cases} > 0 & \text{if } 2\alpha < 1 \rightarrow \text{I} \\ = 0 & \text{if } 2\alpha = 1 \rightarrow \text{II} \\ < 0 & \text{if } 2\alpha > 1 \rightarrow \text{III,} \end{cases}$$

see Figure 5.2. In case II the flow is zero and does not depend on the scaling of the system. The value of the coupling strength that leads to a vanishing flow is called a fixed point. That means that the system looks the same at all length scales, one can zoom in or out while the system does not change. This contradicts the statement that every system has an intrinsic length, called correlation length. One must conclude that the result of case two can only be true for two possible correlation lengths

$$\xi = 0 \quad \text{or} \quad \xi = \infty. \quad (5.17)$$

Since the case of an infinite large correlation length marks a second order quantum phase transition, the fixed point of the flow is identified as a critical value

$$2\alpha_c = 1 \rightarrow \alpha_c = \frac{1}{2}. \quad (5.18)$$

This result was derived for the action in the charge picture of eq. (5.3). The TB paths, and therefore the interactions of the charges, of a particle tunneling forth and back between two neighboring wells in a lattice or a double well do not differ. Hence the above result is true for the microscopic double well and the lattice, respectively. On the contrary the comparison of the coupling strengths for both cases yielded

$$\alpha_{\text{double}}^{\text{mic}} = 2\alpha_{\text{lattice}}^{\text{mic}}. \quad (5.19)$$

We have to conclude that the critical values for the dissipative quantum phase transitions read

$$\alpha_{\text{c,lattice}} = \frac{1}{2}, \quad \alpha_{\text{c,double}} = 1. \quad (5.20)$$

Since we describe the system in analogy to a Coulomb gas, we can use the terminology of a gas to interpret the result physically. In this case the parameter λ can be identified as the fugacity of the gas

$$e^{-\beta\mu}, \quad (5.21)$$

where μ is the chemical potential, which controls the number of particles in the system. Analogous the phases of eq. (5.17) can be related to

$$\begin{aligned} \text{phase I : } e^{-\beta\mu} \rightarrow 1 &\Rightarrow \text{gas is not dilute: many free kinks/antikinks,} \\ \text{phase III : } e^{-\beta\mu} \rightarrow 0 &\Rightarrow \text{gas is very dilute: nearly no free kinks/antikinks.} \end{aligned} \quad (5.22)$$

In order to check the calculation we reproduce the results for the critical coupling strength of the spin-boson-system. We thus insert the effective action of eq. (4.52) into the partition function of

eq. (5.2). The calculation is, except for the replacement of the influence action, identical to that of the delta-system. Only in eq. (5.10) the charge interaction term $\sum_{i,j}^n e_i e_j$ has to be replaced by $-n$. Consequently the result for the critical value differs from the result in (5.18) by a factor 2

$$\alpha_c^{\text{SB}} = 1. \quad (5.23)$$

This result can be compared with the results of Schmid [5] and Bulgadaev [6] for the SB-double-well and the lattice, respectively. We therefore have to replace the TB constant and the Planck constant according to

$$q_0 \rightarrow 2\pi \quad \text{and} \quad \hbar \rightarrow 1. \quad (5.24)$$

Then the coupling strength becomes

$$\alpha_c^{\text{SB}} = 1 = \frac{\eta_c q_0^2}{2\pi \hbar} \rightarrow \frac{\eta_c (2\pi)^2}{2\pi} = 1, \quad (5.25)$$

and we obtain for the critical dissipation coefficient

$$\eta_c^{\text{SB}} = \frac{1}{2\pi}. \quad (5.26)$$

This coincides with the results of [5, 6]. In the SB-system there is obviously no difference between the double well and the lattice.

Summary and outlook

In chapter 3 the mapping between the microscopic Hamiltonian and the spin-boson Hamiltonian yielded the coupling strengths for the microscopic system. The comparison of the results showed that the coupling strengths of the microscopic double well and the lattice are different. We argued that this might arise from a difference in the coupling, since the particle in the microscopic double well couples to the antisymmetric mode of the bose tubes. Another result of the mapping was the characterization of the dissipation as ohmic by calculating the spectral function. In chapter 4 we used the path integral formulation of statistical mechanics to derive the effective action, that does not explicitly depend on the environment. We reformulated the effective action in the Coulomb gas model for the case of the spin-boson-system. In this formulation the coupling to the environment is encoded in the interactions between the charges. Starting with the Coulomb gas model we considered the interactions between the charges for an arbitrary path in the microscopic system and derived the effective action in the Coulomb gas formulation. The evaluation of the sum over the interactions in both cases, the spin-boson-model and the microscopic model, revealed that there are twice as much negative charge interactions in the microscopic system as in the spin-boson system. We can therefore conclude that the coupling to the localized bose tubes does alter the influence of the environment. In chapter 5 we investigated the partition function in the Coulomb gas formulation by applying the renormalization group method. With the help of the rescaling we derived the flow equation of the fugacity and determined the critical coupling strength that marks the dissipative quantum phase transition. As the mapping resulted in a difference between the coupling strengths, the critical value for the microscopic double-well is $\alpha_c = 1$ and for the lattice $\alpha_c = \frac{1}{2}$, respectively. From a physical point of view, one would expect that the size of the system does not affect the critical behavior of the system, as it was shown by Schmid [5] and Bulgadaev [6] for the spin-boson double well and lattice, respectively. It would be interesting to investigate further the origin of this difference. In the microscopic case the positive and negative flow of the fugacity suggests, that the two phases can be characterized by their diluteness. For small coupling strengths the gas is very dense, and there are many free kinks and antikinks in the gas. For coupling strengths bigger than the critical value the gas is very dilute and there are nearly no free kinks and antikinks. In order to identify these phases in analogy to the result of Schmid [5] as diffusive and located phases one would have to calculate the quantum transport.

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