Chapter 10

Non-equilibrium physics

Learning goals

- Why are non-equilibrium aspects important to cold atoms?
- What is special about isolated systems?
- What is a collapse and revival phenomenon?
- What is a bath and how can it be modeled?

10.1 Overview

In (quantum) statistical mechanics we are usually given a Hamiltonian $\hat{H}$ that should describe the system and we are faced with the problem to calculate expectation values relevant for a given experimental measurement. Generically we assume to be either in the ground state $|\psi_0\rangle$ or in a thermal state $\hat{\rho} = e^{-\beta\hat{H}}$, where $1/\beta = k_{\mathrm{B}}T$. In both cases the expectation values are given by

$$\langle \hat{A}(t)\rangle = \mathrm{Tr}\left[\hat{A}(t)e^{-\beta\hat{H}}\right] \qquad \text{or} \qquad \langle \hat{A}(t)\hat{B}(t')\rangle = \mathrm{Tr}\left[\hat{A}(t)\hat{B}(t')e^{-\beta\hat{H}}\right]. \qquad (10.1)$$

These simple formulas are somewhat deceiving. Either we need to be strictly in the ground-state ($\beta \to \infty$), or we assume that the system reached a thermal equilibrium with some "large" bath that provided the notion of a temperature T. Neither of these assumptions are generically fulfilled in experiments with ultra-cold atoms.[1]

In the present chapter we are looking into two different situations where one can capitalize on this specific properties of quantum gases. First, if there is no good bath attached which can thermalize our system, we have the unique opportunity to observe pristine quantum many-body dynamics. We can track the coherent evolution of some complicated many-body state and observe its intrinsic dynamics. In a solid state system such a coherent quantum dynamics is often contaminated by the influence of other, unwanted, degrees of freedom.

In a second example we are studying how one can re-introduce a *custom-tailored* bath. Given the high degree of control on the Hamiltonian of the system, one can try to extend this control to the non-unitary evolution of an open system. Indeed we will see how using the specific tailoring of a bath, one can prepare specific ground states of model Hamiltonians.

The present discussion of non-equilibrium phenomena in general and their appearance in quantum gas experiment is far from being exhaustive. The purpose of this chapter is to give a flavor of the physics in a non-equilibrium setup using two simple examples.

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[1]Which raises the questions why we call them cold...?

10.2 Isolated systems: pure quantum dynamics

In a closed quantum systems the dynamics of many-body system can be observed without the contamination from other degrees of freedom. This is particularly important for the observation of dynamical properties that involve excited states. The case of *repulsively bound states* is a prime example.

10.2.1 Repulsively bound pairs

Let us consider a one-dimensional Bose Hubbard model

$$H = -t \sum_i \hat{a}_i^\dagger \hat{a}_{i\pm 1} + \frac{U}{2} \sum_i \hat{n}_i(\hat{n}_i - 1). \tag{10.2}$$

For the discussion of repulsively bound pairs we are interested in the two-particle problem. To this end, we want to switch back to a first quantized description as we restricted to a specific particle number. We are writing for the two particle wave function $\psi(x, y)$, where x (y) is the discrete coordinate of the first (second) particle, respectively. The Schrödinger equation now reads

$$H\psi(x, y) = \left[-t\tilde{\Delta}_x - t\tilde{\Delta}_y + U\delta_{x,y} \right] \psi(x, y) = E\psi(x, y). \tag{10.3}$$

The first two terms are the discrete Laplace operators

$$\tilde{\Delta}_x \psi(x, y) = \psi(x + 1, y) + \psi(x - 1, y) - 2\psi(x, y), \tag{10.4}$$

$$\tilde{\Delta}_y \psi(x, y) = \psi(x, y + 1) + \psi(x, y - 1) - 2\psi(x, y) \tag{10.5}$$

and the last term encodes that the particles only interact when they are on the same site. The Schrödinger equation does not depend on the center of mass $R = (x + y)/2$, so we write

$$\psi(x, y) = e^{iKR}\psi_K(r) \qquad \text{with} \qquad r = x - y. \tag{10.6}$$

Inserted into the the Schrödinger equation we obtain

$$\left[-2t\tilde{\Delta}_{r,K} + E_K + U\delta_{r,0} \right] \psi_K(r) = E\psi_K(r), \tag{10.7}$$

where

$$\tilde{\Delta}_{r,K} \psi_K(r) = \cos\left(K/2\right) \left[\psi_K(r + 1) + \psi_K(r - 1) - 2\psi_K(r) \right], \tag{10.8}$$

and the center of mass kinetic energy is given by

$$E_K = 4t[1 - \cos(K/2)]. \tag{10.9}$$

The free ($U = 0$) part is solved with a Fourier-transformation $\psi_K(k) = \frac{1}{\sqrt{N}} \sum_r \exp(irk)\psi_K(r)$ which yields

$$\left\{ \underbrace{4t\cos(K/2)[1 - \cos(k)]}_{\epsilon_{K,k}} + E_K \right\} \psi_K(k) = E\psi_K(k). \tag{10.10}$$

We are now ready to tackle the interacting problem.

Lippmann-Schwinger equation

We cast equation (10.3) into the following form

$$\left[2t\tilde{\Delta}_{r,K} - E_K + E \right] \psi_K(r) = \underbrace{U\delta_{r,0}\psi_K(r).}_{\text{"source term"}} \tag{10.11}$$

In the standard way we solve for the Greens function where we replace the source term with a simple point source

$$\left[2t\tilde{\Delta}_{K,r} - E_K + E \right] G(r, E, K) = \delta_{r,0}. \tag{10.12}$$

After a Fourier-transform $(r \to k)$ and making use of (10.10) we find

$$G(k, E, K) = \frac{1}{E - (E_K + \epsilon_{K,k}) + i\eta}. \tag{10.13}$$

Equation (10.11) can now be solved via a convolution of the actual source $[U\delta_{r,0}\psi_K(r)]$ with the Greens function. As usual we can add a solution of the "free" part which is here just $\exp(ikr)$. With this we arrive at the Lippmann-Schwinger equation

$$\psi_K(r) = e^{ikr} + \int dr' G(r - r', E, K)\delta_{r',0}U\psi_K(r'), \tag{10.14}$$

with $G(r, E, K) = \int \frac{dk}{2\pi} G(k, E, K)e^{-ikr}$. Owing to the delta function in the source term the above equation reduces to

$$\psi_K(r) = e^{ikr} + G(r, E, K)U\psi_K(0). \tag{10.15}$$

This is still a non-trivial equation for the wave function $\psi_K(r)$. However, we can set $r = 0$ to find

$$\psi_K(0) = 1 + G(0, E, K)U]\psi_K(0) \quad \Rightarrow \quad \psi_K(0) = \frac{1}{1 - UG(r = 0, E, K)}. \tag{10.16}$$

Putting everything together we find for the full solution

$$\psi_K^{\text{scattering}}(k) = \delta_{k,k'} + G(k', E, K)\frac{U}{1 - UG(r = 0, E, K)}. \tag{10.17}$$

The first part describes an incoming wave at k'. The second part is the scattering part int momentum k. In addition to the scattered wave, there is a resonance at $1 - UG(r = 0, E, K) = 0$, where we can neglect the first part. Such a solution which does not depend on the incoming wave is called a bound state. The question is now for which energy E and total momentum K does such a bound state exist. Performing the Fourier transform on the Greens function we arrive at

$$E_{\text{bs}}(K) = 4t + \text{sign}(U)\sqrt{U^2 + 8t^2(1 + \cos(K))}. \tag{10.18}$$

In one dimension, this energy always lies above (below) the two-particle continuum $\epsilon_{K,k}$ for repulsive (attractive) interaction, respectively. Hence, this bound state is stable. For attractive $U < 0$, this comes as no surprise. What is however, the physics of such a bound state for repulsive interactions?

In the presence of a band gap, i.e., on a lattice, the repulsively bound state is stable. If we would like to take a two-particle tower apart, we would have to accommodate the excess energy U into kinetic energy. However, this energy might lie in the band gap. It turns out, that in one dimension, the additional constraint in the preservation of total momentum makes this energy always to lie in the band gap!

Such a repulsively bound pair can only survive if nobody else can carry away the excess energy U. The fact that this bound states have been observed by Winkler et al. in Nature 853, **441** (2006) can be seen as a clear sign of the perfect isolation of cold atomic gases.

10.2.2 Collapse and revival

Another example of such non-equilibrium dynamics arises after a quench (sudden change) from a superfluid deep into a Mott insulator (e.g. to $t = 0$). The super fluid order parameter $\psi = \langle \hat{a} \rangle$ for the ground state at $t = 0$ is clearly zero. What happens to the superfluid order parameter $\psi(\tau)$ as a function of time τ after the quench?

To answer this question we note that the eigenstates of the Hamiltonian $H = \frac{U}{2} \sum_i \hat{n}(\hat{n} - 1)$ are simply given by Fock states

$$H|n\rangle = Un(n-1)|n\rangle. \tag{10.19}$$

In order to track the time evolution after the quench we only need to expand the initial ground state in terms of the new eigenstates

$$\Psi(\tau = 0) = \Psi_{\text{SF}} = \sum_{n_1, n_2, \dots} \alpha_{n_1, n_2, \dots} |n_1, n_2, \dots\rangle. \tag{10.20}$$

The time evolution is now given by

$$\Psi(\tau) = \sum_{n_1, n_2, \dots} \alpha_{n_1, n_2, \dots} e^{i\tau U[n_1(n_1-1) + n_2(n_2-1) + \cdots]} |n_1, n_2, \dots\rangle. \tag{10.21}$$

From the above equation we immediately see that after time $\tau = \frac{2\pi}{U}$ the exponential only contains multiples of 2π and hence the original wave function is restored! Consequently, also the superfluid order parameter ψ will be restored to its original value. Such collapse and revival experiments have been reported in Nature 419, **51** (2002).

10.3 Driven-dissipative systems

A very different non-equilibrium aspect of cold atoms can be revealed by the engineering of a suitable bath for quantum gases. In this approach, the absence of a bath and the high level of control on the dynamics of trapped quantum gases can be combined in the design of a suitable artificial bath. In order to understand this we need to be able to describe a system weakly coupled to a bath.

10.3.1 The quantum master equation

Let us start from a system weakly coupled to a bath as described by the Hamiltonian

$$H = H_{\text{sys}} + H_{\text{int}} + H_{\text{bath}}. \tag{10.22}$$

We are now targeting an equation of motion for our system density matrix ρ_{sys} where we don't want to keep track of what is happening to the bath degrees of freedom. Under the following three condition one can derive the quantum master equation

1. The density matrix of the full system at time $t = 0$ can be written as $\rho(0) = \rho_{\text{sys}} \otimes \rho_{\text{bath}}$. In other words, the system and the bath are initially not entangled.

2. $\partial_t \rho_{\text{bath}} = 0$: The state of the bath is not changed by what happens in our system.

3. The time dependent correlation function of the bath are not changed by the coupling to the system, i.e., the bath is much *faster* than the system.

Using these assumptions and considering an interaction Hamiltonian of the form

$$H_{\text{int}} = \sum_{\alpha} \hat{J}_{\alpha}^{\dagger} \hat{O}_{\alpha}^{\text{bath}} + \text{H.c} \tag{10.23}$$

where $\hat{J}_\alpha$ denotes a system operator we arrive at the master equation

$$\partial_t \rho_{\text{sys}}(t) = -i[H_{\text{sys}}, \rho_{\text{sys}}(t)] \tag{10.24}$$

$$- i \sum_\alpha \left[\delta_\alpha \hat{J}_\alpha^\dagger \hat{J}_\alpha + \epsilon_\alpha \hat{J}_\alpha \hat{J}_\alpha^\dagger, \rho_{\text{sys}}(t) \right]$$

$$+ \sum_\alpha K_\alpha \left(\hat{J}_\alpha \rho_{\text{sys}}(t) \hat{J}_\alpha^\dagger - \frac{1}{2} \left\{ \hat{J}_\alpha^\dagger \hat{J}_\alpha, \rho_{\text{sys}}(t) \right\} \right)$$

$$+ \sum_\alpha G_\alpha \left(\hat{J}_\alpha^\dagger \rho_{\text{sys}}(t) \hat{J}_\alpha - \frac{1}{2} \left\{ \hat{J}_\alpha \hat{J}_\alpha^\dagger, \rho_{\text{sys}}(t) \right\} \right).$$

The first three terms describe the coherent system evolution, the Lamb- and Stark-shift respectively. The last two terms account for the non-unitary evolution induced by the coupling to the external bath.

Here we tried to argue that quantum gases are generically not connected to a bath. What is now the value of the above equation for our discussion? It turns out, that as much as one can design system Hamiltonians, one can also try to design suitable "jump operators" J_α in order to directly implement a desired non-unitary evolution. This is particularly interesting if the long-time limit of such a designed non-unitary evolution is not some generic mixed state but a well defined pure quantum state. In such a case, one can use a bath to prepare a desired (ground) state. We illustrate this procedure on the example of a recent publication in Nature Phys. 878, **4** (2008).

10.3.2 Bath tailoring

We can write directly a desired Liouvillian

$$\partial_t \rho_{\text{sys}}(t) = -i[H_{\text{sys}}, \rho_{\text{sys}}(t)] + \sum_\alpha K_\alpha \left(\hat{J}_\alpha \rho_{\text{sys}}(t) \hat{J}_\alpha^\dagger - \frac{1}{2} \left\{ \hat{J}_\alpha^\dagger \hat{J}_\alpha, \rho_{\text{sys}}(t) \right\} \right). \tag{10.25}$$

This generically leads to a mixed steady state $[\rho_{\text{sss}} = \rho_{\text{sys}}(t \to \infty)]$. However, under special circumstances, the long time limit can be a pure state $|D\rangle$. This is the case if

1. $|D\rangle$ is a an eigenstate of all jump operators $\hat{J}\dagger|D\rangle = 0$ with eigenvalue 0, and

2. $|D\rangle$ is "compatible" with the unitary dynamics, i.e., $H|D\rangle = E|D\rangle$.

In the language of quantum optics $|D\rangle$ is called a "dark state".

Long-range order by local dissipation

How can we now design a set of jump operators that lead to such a dark state. Consider a Bose-Hubbard model where we set the interaction U to zero. The ground state $|\text{BEC}\rangle$ is given by all particles residing in the $k = 0$ mode $\hat{a}_{k=0}^\dagger \propto \sum_i \hat{a}_i^\dagger$. Hence, if we want to prepare the state $|\text{BEC}\rangle$ via a designed bath, we need to make sure that only states survive where the phase between adjacent sites is set to zero. The following jump operators would do the job

$$\hat{J}_\alpha = \hat{J}_i = (\hat{a}_i^\dagger + \hat{a}_{i+1}^\dagger)(a_i - a_{i+1}). \tag{10.26}$$

Clearly $J_\alpha|\text{BEC}\rangle = 0$ for all α. Moreover, the state $|\text{BEC}\rangle$ is compatible with the unitary dynamics (at $U = 0$). How can we now design such a jump operator in an experiment? Imagine a cubic optical lattice where at each link of the original (system) lattice there is another (high-energy) state available, cf. Fig. 10.1. If we now pump the system with Rabi frequencies $\pm\Omega$ from the lower to the upper "band", the system framed in red constitutes a standard Λ-system. If the particle is allowed to decay back down to the lower band, we indeed deal with a
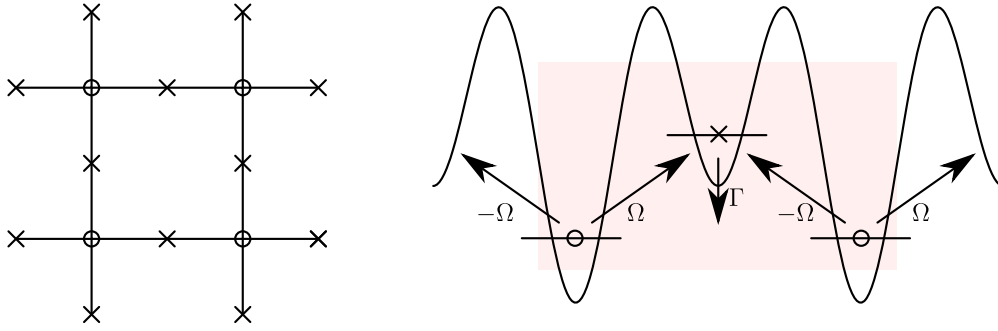
Figure 10.1: Setup for dissipative cooling.

jump operator of the form $C_{\alpha,i,j}\hat{a}_\alpha^\dagger(\hat{a}_i - \hat{a}_j)$. Two problems need to be addressed: (i) How can the particle fall back down to the lower sites. (ii) How are the coefficients $C_{\alpha,i,j}$ related to the desired jump operator in Eq. (10.26).

The first problem can be solved by immersing the whole setup into a big (not necessarily $T = 0$) Bose Einstein Condensate. The particles falling down can then transfer their excess energy to a Bogoliubov excitation of the "big" condensate. The details of the coupling then also encode the properties of the coefficients $C_{\alpha,i,j}$. However, the details are not crucial, as long as the local antisymmetric combination is pumped up, and hence $|\text{BEC}\rangle$ is a dark state. More details about this setup are discussed in Nature Phys. 878, **4** (2008).

What was the magic of this bath tailoring? The crucial aspect was that we found a local pump, where antisymmetric phase configurations on a lattice are removed by the jump operator. The resulting dark state, however, had a long-range phase coherence. Hence, via local operators we managed to prepare a long-range correlated state. Following the aforementioned publication, various proposals were formulated where the long-range correlated state is much more complicated than the $|\text{BEC}\rangle$ discussed here. This includes d-wave superconducting fermion systems or topological p-wave superconductors.