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Localization in disordered bosonic insulators with strong short-range interaction

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Contents

Abstract

This thesis consists of two parts. The first is a small introduction into the theory of Anderson localization, accompanied by the description of a recent experiment that shows the relevance of the concepts.

The second part is the actual project. A new technique is introduced, which uses Hubbard operators. It is made clear why this technique is necessary and some basic properties of Hubbard operators are discussed. The classical Wick's theorem is extended to operators with non-trivial commutation and anticommutation relations. A scheme is introduced to keep track of all created diagrams. Then it used to calculate single particle Green's functions in the forward scattering approach for fermions and hard-core bosons on a disordered lattice. Some calculations are made to improve upon the results of forward scattering by inclusion of real space and Fock space deviations. It is argued that strong interactions tend to supress the transport of bosons. Possible experimental realizations are then considered.

Acknowledgment

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Chapter 1

Introduction to Anderson Localization

In this section I present a brief introduction to Anderson localization transition. I illustrate the connection to very recent experiments with cold atoms and ultra sound, that shows in a very impressive way, that Anderson localization is a universal concept.

1.1 Quantum Localization

The Anderson location is a very peculiar quantum phenomenon present in disordered media. The concept of it was introduced by Anderson [4] in 1958. It is truly astonishing, that after more then five decades after its introduction, Anderson localization is still a hot research topic in physics and mathematics and is used in ways not even Anderson himself could have imagined. [1] For a general notion of localization I follow the review article by Evers and Mirlin [5] and the books by Haake [1], Efetov [2] and Stöckmann [3].

One of the classic results of quantum physics is the Bloch theorem. It states that electrons in a periodic crystal form so called Bloch waves, delocalized waves that are periodically modulated and extend all over the crystal.

How are things changed in a disordered system? A good example is given by the Anderson's hopping model [4]. One considers a one dimensional chain of equidistant sites with a random on site potential. The hopping of particles is described by a hopping amplitude t_r that depends only on the difference between sites and decreases typically fast with r. Then the wave amplitudes ψ_i, corresponding to the lattice sites $\{i\}$, for a particle with energy E obeys the Schrödinger equation on a lattice

$$U_m\psi_m + \sum_r t_r\psi_{m+r} = E\psi_m. \qquad (1.1)$$

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[1] Quote from Andersons Nobel lecture, 1977: *"Localization [..], very few believed it at the time, and even fewer saw its importance, among those who failed to fully understand it at first was certainly its author. It has yet to receive adequate mathematical treatment, and one has to resort to the indignity of numerical simulations to settle even the simplest questions about it."*

Here U_m is the on-site potential of lattice site m, typically drawn from a density $\rho(U_m)$. If the potentials U_m would be periodic, i.e. $U_m = U_{m+K}$, then Bloch's theorem would have to be fulfilled and nothing new happens. However, at least for the one dimensional case one can easily demonstrate that a new phenomena has to happen. Let's assume, that only nearest neighbor tunneling elements are non-zero, e.g. $t_1 = t, t_i = 0$ for $i > 1$. In one space dimension, the Schrödinger equation (1.1) can be brought into a particular convenient form, connecting the wave amplitudes of the lattice sites to their neighbors.

$$\begin{pmatrix} \psi_{m+1} \\ \psi_m \end{pmatrix} = \begin{pmatrix} (E - U_m)/t & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \psi_m \\ \psi_{m-1} \end{pmatrix} = F_m \begin{pmatrix} \psi_m \\ \psi_{m-1} \end{pmatrix} \qquad (1.2)$$

This is a matrix equation involving random, unimodular 2×2 matrices F_m. Unimodular means in this case that $|\det F_m| = 1$. Under these conditions Furstenberg's theorem[6] applies, which states that

$$\lim_{N \to \infty} \frac{1}{N} \ln \mathrm{Tr} \left\{ F_N F_{N-1} \dots F_2 F_1 \right\} \equiv \gamma > 0. \qquad (1.3)$$

Now given that the initial amplitudes ψ_0, ψ_1 are known, one can find the amplitudes at different lattice sites by

$$\begin{pmatrix} \psi_{m+1} \\ \psi_m \end{pmatrix} = F_N F_{N-1} \dots F_2 F_1 \begin{pmatrix} \psi_1 \\ \psi_0 \end{pmatrix}. \qquad (1.4)$$

So by applying Furstenberg's theorem one can see, that far away from the initial sites, the wave amplitudes must behave as $\exp[\pm m\gamma]$ (for almost all sites). Since the particle amplitudes are normalized, unlimited growth in one direction is not allowed and one must have localization around a site with an exponentially decreasing tail. Also, the eigenenergies of the Hamiltonian cannot form a continuum, because only special values of E let the wave function decrease in both directions. The factor γ is called the Lyapunov exponent of the random map generated by (1.2). Its physical interpretation is that of an inverse localization length ξ. The wave function centered around site i can be described far away from the center by

$$\psi_m^i \sim e^{-|i-m|/\xi} \text{ for } |i - m| \to \infty. \qquad (1.5)$$

This result is drastically different from the Bloch functions with their continuous bands of eigenenergies. Localization occurs even under arbitrary small disorder. But it is easy to see why localization has to occur. Even if the probability for a scattering event is small, in one dimension this leads to a complete change of direction of the wave and it can return to its fixed point. All the complex amplitudes of the waves have to add up, which then means localization. The result that in one dimension always localization occurs was first argues by Mott and Twose [14] and later proven by Berezinsky [15] using diagrammatic technique. So one can define Anderson Localizations as Quantum Mechanical localizations induced by disorder. They have tremendous effects on the properties of materials. Originally only the Anderson metal-insulator transition due to disorder was considered. Later, localization was found in other systems with wave character as well, like the absence of diffusion in atomic matter waves [7, 8, 9, 44] or the localization of ultra sound [10] and light waves [11, 12, 13]. In one dimension and uncorrelated disorder, localization is always present. But what happens in higher dimensions?

1.2 The One-parameter scaling hypothesis

A milestone in the theory of Anderson localization were the scaling arguments by Thouless [32]. He predicted that for wires, even in larger space dimensions, the resistivity increases exponentially given that the wire is longer than a critical length $L_c \sim p_0 Al$, p_0 is the Fermi momentum, A the cross section of the wire and l the mean free path. This is remarkable since all systems behave the same, as long as they have a one-dimensional geometry. At the critical length L_c they share the same resistivity ($\approx 10k\Omega$). An intergral part of Thouless reasoning was, that the behaviour of the system depends only on the conductance alone. Buildung up on this idea, another important contribution to the theory of Anderson localization was made by the "Gang of Four" [33]. They generalized the idea that the behaviour of the conductance, depends only on the conductance itself. They argued that for a block of disordered metal in d dimensions, that is made out of b blocks of length L in each direction, the relation

$$g(bL) = f(b, g(L)) \tag{1.6}$$

must hold. In differential form and in the limit $b \to 1$, this becomes a relation for the scaling function β that describes how the conductance changes under a change of length

$$\beta = \frac{d\ln g}{d\ln L} = \beta(g), \qquad g = \frac{\hbar}{e^2} G. \tag{1.7}$$

This scaling function depends on the dimensionality of the system and one can determine the asymptotic behaviour. Consider a hypercube of size L^d. For small conductances, i.e. the insulating regime, the conductance is an exponentially decaying function, because the wavepackets are localized

$$g = g_0 e^{-\alpha L} \to \beta(g) = \lim_{g \ll 1} L \frac{d\ln g}{dL} = -\alpha L = \ln\left(\frac{g}{g_0}\right). \tag{1.8}$$

This result is independent of the dimension of the system. More interesting is the limit of large conductances. Here one knows the classical limit, namely Ohm's law, given by

$$G(L) = \sigma L^{d-2}, \sigma = \frac{ne^2\tau}{m} = \frac{ne^2 l}{\hbar k_f}, \tag{1.9}$$

a result that follows from Drude theory. Here n is the electron density, τ the transport time and l the mean free path of the electron. At large conductances, the β-function thus behaves as

$$\lim_{g \to \infty} \beta(g) = d - 2. \tag{1.10}$$

If one assumes smoothness and monotony of the β function, one can interpolate between these limits. The result is sketched in (1.1).

Because the scaling function describes how the system scales under increasing conductance, the sign of the β function tells whether one is in the insulating
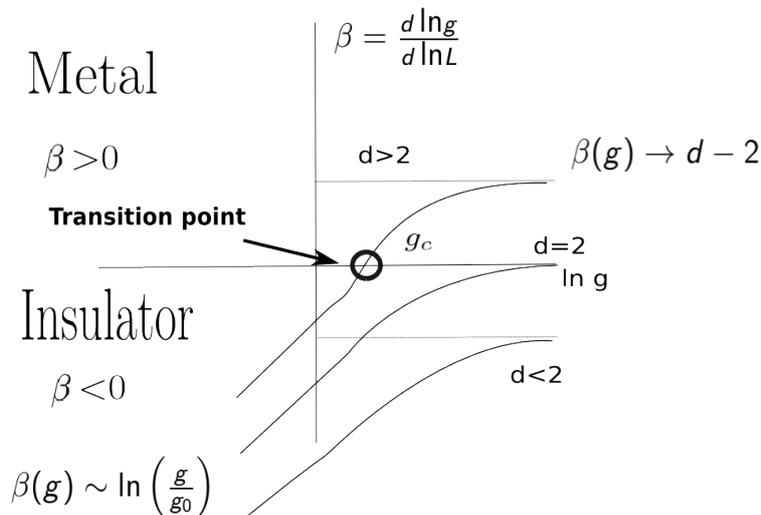
Figure 1.1: The β function in one, two and three dimensions.

($\beta < 0$) or conducting regime ($\beta > 0$). As shown earlier, in one dimension and uncorrelated disorder there is only an insulating regime, so it is in two dimension. However, for large conductances, the β function in two dimensions approaches zero and one obtains quasi-metallic behaviour (for the case of uncorrelated disorder). In three dimensions and above, one has clearly a crossing at the unstable fixpoint $\beta = 0$ which is accompanied by an Anderson transition from the insulating into the metallic state at a critical conductance g_c.

Later it was argued, that the one-parameter scaling hypothesis should be replaced by a scaling hypothesis for a distribution function of conductances [16, 17, 18, 19]. Nonetheless, localization in two dimensions and weak disorder was proven analytically and numerically [20]. However, the one-parameter hypothesis was a milestone in the field and it is believed that the results hold generally. In order to clearly observe the Anderson transition experimentally, one has to explore higher dimensional systems ($d > 2$). Solid state systems are not an optimal choice, because the disorder is difficult to tune and localiation is hard to observe [21]. However, creating disordered potentials for large dimensions is difficult (even 3D disorder for cold atomic matter was only implemented very recently [76]), because our accessible space has only three dimensions. An additional insight is needed to make these systems experimentally feasible. Section (1.4) and (1.5) will deal with this problem in more detail.

1.3   Interference in disordered systems

So far it was not explained, what makes dimension one and two so special. With the classical Drude model the disordered metals should obey the Boltzmann equation, so they were expected to be conductors. In order for the behaviour to

change so drastically, the quantum mechanical corrections must diverge. In this section a qualitative picture is presented that was first suggested by Khmelnitskii and is based on several works of the pioneers of this field[**?**, 24].

The motion of electrons in the limit of weak disorder $p_0 l \gg 1$ can be described by path integrals. Consider the motion between two points r_1 and r_2. In a classical picture, simply all probabilities of all possible paths are added. However the rules of quantum mechanics are different. The total probability for the event is the square of the total amplitude, which is the sum of all paths. If A_i denotes the complex amplitude of path i, then the toal probability P of propagation is

$$P = \left| \sum_i A_i \right|^2 = \sum_i |A_i|^2 + \sum_{i \neq j} A_i A_j^*. \tag{1.11}$$

The first term is the classical sum over all probabilities of the individual paths $P_i = |A_i|^2$. The second term is an additional interference term between different paths. For typical paths (see figure (1.2,a)) this term does not contribute, because most paths differ in length and disorder potential, such that the phase $\phi = \hbar^{-1} \int_1^2 \vec{p} d\vec{r}$ aquired over each is random. This means that the overall sign changes from term to term. Summing over all paths, this term oscillates fast and becomes negligible.

However, not all paths are so uncorrelated. There is the possibility of self-intersecting paths (see figure (1.2,b)). To each self-intersecting path corresponds another one with the same shape and length, where the only difference is the direction in which the loop is traversed.
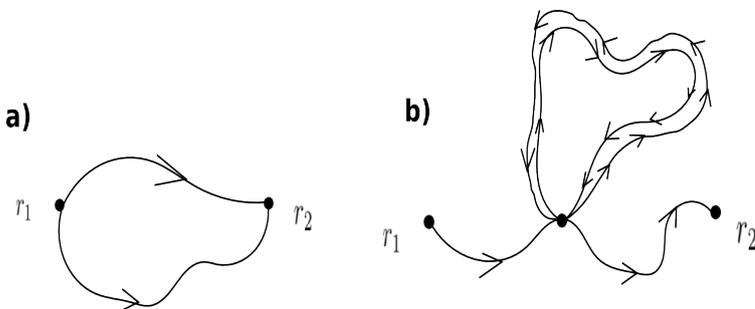
Figure 1.2: Paths with a) and without b) self crossing sections

When a loop is transversed in the opposite direction, the $\vec{p}$ and $d\vec{r}$ aquire both a minus sign and the overall phase is the same, provided that there is time-reversal symmetry. This means that for these two paths

$$|A_1 + A_2|^2 = |A_1|^2 + |A_2|^2 + A_1 A_2^* + A_2 A_1^* = 4 |A_1|^2, \tag{1.12}$$

because their total amplitudes are the same. This means, that the quantum mechanical probability for this path is enhanced compared to the classical probability. Paths with many loops or bigger loops ($d > 1$) have a higher probability to occur than paths with no loops at all. For a closed path, all trajectories have

a time-reversed counterpart and hence the return probability is high. If one-loop-paths are the leading contribution one speaks of weak localization, even though real localiation has not occured yet.

These arguments did not depend on the dimensionality so far. But the ratio of self-intersecting paths to all paths depends on the dimensionality. It is well known, that for an unbiased random walk on a lattice, the return probability in one and two dimensions is unity, whereas it is less in higher dimension. To argue physically, the path of an electron is not an infinitely thin line, but rather a tube with thickness of the order of the de Broglie wave-length $\lambda \sim \hbar/p_0$. So in the time interval dt the volumeelement $v\lambda^{d-1}\,dt$ is traversed. This is roughly the space the electron takes up in its travel. Now the probability for self-intersection can be seen as the ratio of space the electron takes up and the space the electron could have reached by moving diffusively. In classical diffusion the length in one direction a particle on average moves is given by $r = \sqrt{D_0 t}$ for $t >> \tau$, $D_0 = v_0^2 \tau/d$ is the classical diffusion constant and v_0 the Fermi velocity. The diffusively availabe space for a particle starting at the origin at $t = 0$ is then in d dimensions $(D_0 t)^{d/2}$ at time t. One can argue that for fermions, the relative loss of conductivity compared to the classical conductivity $\sigma_0 = ne^2\tau/m$, where n is the electron density, m the electron mass and τ the mean free time, is proportional to the return probability, so that

$$\frac{\Delta\sigma}{\sigma_0} \sim -\int_\tau^{\tau_\phi} v\lambda^{d-1}\left(D_0 t\right)^{d/2} dt. \qquad (1.13)$$

The lower limit of integration is the mean free time because only for larger times the diffusion picture is meaningful. The upper bound is the time of phase coherence t_ϕ, because only coherent waves can interfere constructively or destructively. Coherence can only be destroyed example by inelastic scattering with phonons.. For low temperatures, inelestic scattering becomes less and less likely so that for $T \to 0$, $t_\phi \to \infty$. Equation (1.13) is convergent and finite for $d \geq 3$, but divergent for $d = 1, 2$. This means, that in these low dimensions, quantum effects always have a dominating effect.

The picture of self-intersection paths can help to get an intuitive understanding of how magnetic fields can influence systems with weak localization. However the general theory of the influence of magnetic fields on localization is vast and not all questions are answered. In this section we consider the influence of magnetic fields on self-intersecting paths. In magnetic field $\vec{H}$, the two time-reversed paths do not have the same amplitude anymore. Instead, the magnetic field induces a phase difference between these paths. In a magnetic field, the momentum is shifted by the vector potential $\vec{p} \to \vec{p} - (e/c)\vec{A}$, with $\vec{\nabla} \times \vec{A} = \vec{H}$. The phase shift is then

$$\Delta\phi_H = \frac{2e}{c\hbar} \oint \vec{A}d\vec{l} = 2\pi\frac{\phi}{\phi_0}. \qquad (1.14)$$

ϕ is the magnetic flux trough the loop and $\phi_0 = ch/e$ is the flux quantum. This means, that at large magnetic fields, the constructive interference is destroyed between the self crossing paths. So for electrons, magnetic fields lead to an increase in conductivity, as first found by Altshuler et al. [34, 35].

Because coherence is destroyed between paths, one can introduce the magnetic coherence time in equation (1.13). When the phaseshift is of the order of the

flux-momentum, then the coherence is destroyed. The average length scale of the loop is again given by $\sqrt{D_0 t}$, so that the average magnetic flux going trough the loop is $\phi = H D_0 t$. This means that

$$\tau_H \sim \frac{\phi_0}{H D_0} \sim \frac{l_H^2}{D_0}, \tag{1.15}$$

where $l_H = \sqrt{c\hbar/2eH}$ is the magnetic length. It depends on the temperature, whether τ_ϕ or τ_H is the time scale over which coherence is destroyed. This in return gives a critical magnetic field $H_c = \phi_0/(D_0 \tau_\phi)$, above which magnetic effects are dominant.

This gives an intuitive picture of how magnetic fields affect electron dynamics for weak disorder. In general this is however not true. For special geometries and other symmetries quite different behaviour can be observed. A famous example is the fluctuation of resistance in a metallic cylinder with an magnetic flux passing it [25, 26, 27]. Magnetic impurities can actually change the sign of the magnetic correction and lead to a positive magnetoresistance for fermionic systems [28] [29].

1.4 The Kicked Rotator in one Dimension

A very interesting model for the study of Anderson localization is the periodically kicked rotator. It is closely related to Anderson's model. Because it is a model that displays classical chaos, it is perfect to study the influence of the quantum nature on the behaviour of a physical system. The periodically kicked rotator is also a minimalistic model for several experimentally accesible systems. Another advantage of this model is its simplicity. The phase space consists only of two variables p and θ, connected by the canonical commutation rule

$$[p, \theta] = \frac{\hbar}{i}. \tag{1.16}$$

These variables evolve by a periodically driven Hamiltonian

$$H(t) = \frac{p^2}{2I} + \lambda \frac{I}{\tau} V(\theta) \sum_{n=-\infty}^{\infty} \delta(t - n\tau). \tag{1.17}$$

The Hamiltonian contains several physical parameters; the moment of intertia I, the kicking period τ and a dimensionless kicking strength λ. The potential $V(\theta)$ is a 2π-periodic function in θ. For simplicity one can take V to be $\cos(\theta)$. The only relevant control parameter of the problem is the kicking strength λ and one can set $I, \hbar$ and τ to one.

Since dynamics is periodic in time, the time evolution of the variables happens in discrete steps. This means that the time evolution can be split into seperate steps of size τ, each with the same time evolution operator. The evolution operator for this stroboscopic problem is called a Floquet operator and it fulfills the equation

$$\psi(t+1) = F\psi(t), \qquad F = e^{i\lambda V} e^{-ip^2/2}. \tag{1.18}$$

One sees, that the right factor $e^{-ip^2/2}$ is responsible for the ballistic rotation of the rotator, while the first $e^{i\lambda V}$ factor describes the instantaneous kick. One can

also apply this time evolution to the variables in the Heisenberg representation and obtain discrete-time Heisenberg equations

$$p_{t+1} = p_t - \lambda V'(\theta_{t+1}) \tag{1.19}$$

$$\theta_{t+1} = \theta_t + p_t \tag{1.20}$$

These relations holds also for the classical problem of a kicked rotator, but with classical variables.

What would one expect classically for large kicking strength? In that case, the average momentum becomes larger and the angular variable moves faster. Since θ is 2π periodic, it will cover the whole interval $[0, 2\pi]$ evenly. For large enough kicking strength, subsequent θs will seem independent of each other. Then the kicking becomes a statistical process with no kick-to-kick memory. The force from each kick is $-V'(\theta_t)$ and independent of the previous one. The time evolution of the momentum variable can then be approximated by

$$p_t = p_0 - \sum_{\nu=1}^{t} \lambda V'(\theta_\nu). \tag{1.21}$$

Because of the definition $V = \cos(\theta)$, the average momentum transfer per kick is zero

$$\overline{p_t} = \overline{p_0} - \sum_{\nu=1}^{t} \lambda \overline{V'(\theta_\nu)} = \overline{p_0}. \tag{1.22}$$

However, the mean square of the momentum grows linearly

$$\overline{p_i^2} = \overline{p_0^2} + \sum_{\mu,\nu=1}^{t} \lambda^2 \overline{V'(\theta_\mu) V'(\theta_\nu)} \tag{1.23}$$

$$= \overline{p_0^2} + \left(\lambda^2 \frac{1}{2\pi} \int_0^{2\pi} d\theta \, V'(\theta)^2 \right) t. \tag{1.24}$$

This is a diffusion equation and must happen, because the noise at different times is not correlated $\overline{V'(\theta_\mu) V'(\theta_\nu)} = \delta_{\mu\nu} \overline{V'(\theta)^2}$. The diffusion constant is given by

$$D = \frac{\lambda^2}{2\pi} \int_0^{2\pi} d\theta V'(\theta)^2 = \frac{\lambda^2}{2} \tag{1.25}$$

whereas the value of $D = \lambda^2/2$ is specific for the model $V = \cos(\theta)$. To sum it up, in the classical periodically kicked oscillator one has for large enough kicking strength a diffusion in momentum space. This can be for instance done numerically and indeed, for $\lambda \geq 1$ one has quasi diffusive behaviour which is equivalent to chaos,,since very close points in phase space evolve away from each other. To prove this, one can linearize the full classical map (*Chirikov's standard map*[30])

$$p_{t+1} = p_t + \lambda \sin \theta_{t+1} \tag{1.26}$$

$$\theta_{t+1} = (\theta_t + p_t) \bmod (2\pi). \tag{1.27}$$

The linearization gives

$$\begin{pmatrix} \delta p_{t+1} \\ \delta \theta_{t+1} \end{pmatrix} = \begin{pmatrix} 1 + \lambda \cos \theta_{t+1} & \lambda \cos \theta_{t+1} \\ 1 & 1 \end{pmatrix} \begin{pmatrix} \delta p_t \\ \delta \theta_t \end{pmatrix} \equiv M_t \begin{pmatrix} \delta p_t \\ \delta \theta_t \end{pmatrix}. \tag{1.28}$$

Since the angular variable is quasi random, M_t is a random unimodular map and Furstenbergs theorem 1.3 applies. This means that for the classical map a positive Lyapunov exponent exists (i.e. chaotic behaviour).

In a quantum mechanical setting the behaviour is quite different. One knows that one can separate the time evolution into two parts, the ballistic motion and the kick. Superscripts "$\mp$" denote a time event right before and right after a kick. Using again the Floquet operator of time evolution one finds

$$\left| \Psi^+(t+1) \right\rangle = F \left| \Psi^+(t) \right\rangle, t \in \mathbb{N} \qquad (1.29)$$

$$\left| \Psi^-(t) \right\rangle = \mathrm{e}^{-iH_0} \left| \Psi^+(t-1) \right\rangle, \qquad H_0 = \frac{p^2}{2} \qquad (1.30)$$

The ballistic motion is best described in terms of its constants, i.e. in a momentum representation

$$p \left| n \right\rangle = n \left| n \right\rangle \qquad (1.31)$$

$$n = 0, \pm 1, \pm 2, \ldots. \qquad (1.32)$$

(we recall $\hbar = 1$). The only part of the Hamiltonian that effects a state between kicks is H_0. It acts in such a way on $\left| n \right\rangle$ that

$$H_0 \left| n \right\rangle = \frac{n^2}{2} \left| n \right\rangle. \qquad (1.33)$$

Because the states are diagonal in this representation, the time evolution in between kicks is $\left| n \right\rangle \to \mathrm{e}^{-in^2/2} \left| n \right\rangle$. Now one can expand the states at the different times in terms of this basis

$$\left| \Psi^\pm(t) \right\rangle = \sum_n \Psi_n^\pm(t) \left| n \right\rangle. \qquad (1.34)$$

Using the above mentioned, one knows that $\Psi_n^-(t+1) = \mathrm{e}^{-in^2/2} \Psi_n^+(t)$.
The kick itself is better described in an angular representation

$$\left| \Psi^\pm(t) \right\rangle = \int_0^{2\pi} d\theta \, \Psi^\pm(\theta, t) \left| \theta \right\rangle, \qquad (1.35)$$

since the time evolution during the kick is given by

$$\Psi_n^+(\theta, t) = \mathrm{e}^{-i\lambda V(\theta)} \Psi^-(\theta, t). \qquad (1.36)$$

To describe the full dynamics one has to take into account, that during a kick a transfer between momentum states takes place, i.e.

$$\Psi_m^+(t+1) = \sum_{n=-\infty}^{\infty} J_{m-n} \mathrm{e}^{-in^2/2} \Psi_n^+(t). \qquad (1.37)$$

Here J_{n-m} is the transfer matrix element during the kick and in general given by $J_{m-n} = \frac{1}{2\pi} \int_0^{2\pi} d\theta \mathrm{e}^{i(m-n)\theta} \mathrm{e}^{-i\lambda V(\theta)}$. In the case of $V = \cos\theta$ the Bessel functions are obtained

$$J_n(z) = \frac{1}{\pi i^n} \int_0^\pi d\theta \mathrm{e}^{iz\cos(\theta)} \cos n\theta. \qquad (1.38)$$

Let's analyze the eigenmodes of the total Hamiltonian or in this context eigenstates of the Floquet operator F with quasi energy ϕ.

$$F\left|u^+\right\rangle = \mathrm{e}^{-i\phi}\left|u^+\right\rangle. \tag{1.39}$$

For an eigenequation to be fulfilled, the relation

$$\sum_n J_{m-n}\mathrm{e}^{-in^2/2}u_n^+ = u_m^+, \tag{1.40}$$

must hold. One could also look at the problem, where first the kick happens and then the free motion. This description is denoted by $\left|u^-\right\rangle$ and is related to $\left|u^+\right\rangle$ (with the same quasi eigenenergy) by

$$u^-(\theta) = \mathrm{e}^{i\lambda V(\theta)}u^+(\theta). \tag{1.41}$$

This can again be rewritten by

$$u^-(\theta) = \mathrm{e}^{i(\phi-H_0)}u^+(\theta), \tag{1.42}$$

or in momentum representation

$$u_n^- = \mathrm{e}^{i\left(\phi-n^2/2\right)}u_n^+ \tag{1.43}$$

The next step is to introduce a new Hermitian operator $W = -\tan\frac{\lambda V}{2}$ to parametrize the kicking operator. Then

$$\mathrm{e}^{-i\lambda V} = \frac{1+iW}{1-iW}. \tag{1.44}$$

Instead of looking at u^+ and u^- individually, it is useful to look at their combination

$$\left|u\right\rangle = \frac{1}{2}\left(\left|u^+\right\rangle + \left|u^-\right\rangle\right). \tag{1.45}$$

Since u^+ and u^- are related by the phase relation (1.41), their the linear combination obeys

$$u(\theta) = \frac{u^+(\theta)}{1+iW(\theta)} = \frac{u^-(theta)}{1-iW(\theta)}. \tag{1.46}$$

Because u^- and u^+ have the same eigenvalue of (1.43), $u(\theta)$ must obey the equation

$$\left[1-iW(\theta)\right]u(\theta) = \mathrm{e}^{i(\phi-H_0)}. \tag{1.47}$$

In momentum representation, the above equation transforms to

$$U_m u_m + \sum_{r\neq 0} t_r u_{m+r} = Eu_m, \tag{1.48}$$

with

$$U_m = i\frac{1-\mathrm{e}^{i\left(\phi-m^2/2\right)}}{1+\mathrm{e}^{i\left(\phi-m^2/2\right)}} = \tan\left(\frac{\phi-m^2/2}{2}\right) \tag{1.49}$$

$$E = -W_0. \tag{1.50}$$

Now this looks like the one dimensional Andersons hopping model (1.1). There are however differences. Whereas the on-site energies in the Anderson model are truly random, one has here only a pseudorandom behavior, since the tan is a fast oscillating function. It is proven by Weyl [31], that $\left(\phi - m^2/2\right) \mathrm{mod}(\pi)$ is ergodic in the interval $[0, \pi]$. Further it has uniform density within that interval for the values of $m = 0, \pm 1, \pm 2, \ldots$. The U_m thus have a density $\rho(U)dU = d\phi/\pi$. Since $dU/d\phi = 1 + U^2$, one finds

$$\rho(U) = \frac{1}{\pi\left(1 + U^2\right)}. \tag{1.51}$$

Thus the effective on-site energy is quasi Lorentzian distributed. Another difference is, that the hops can not just happen between nearest neighbors, but the hopping elements fall of exponentially with r. As one can see from the definition of W, the kicking strength λ does not influence the disorder but rather the hopping amplitudes. It is still very similar to the one dimensional Anderson model with uncorrelated disorder, for which one knows that localization is inevitable. The property of localization can be checked numerically and is indeed seen. After a short time of diffusive behaviour till $\tau_{loc} \approx D/2$, the average momentum distribution stops spreading and approaches the equilibrium value of

$$\left\langle p^2\right\rangle (t \to \infty) \to 2\xi^2. \tag{1.52}$$

Thus the whole phenomenology is drastically different in classical and quantum systems. Instead of a diffusion in momentum space there is localization in momentum space. This effect is called *dynamical localization* and the correspondence to Anderson localization were made by Fishman et al. [36], Shepelyansky [37] and Casati et al. [38]. This effect was first implemented in explaining why specific atoms in a microcavity don't ionize, even though the classical threshold radiation is reached [39, 40, 41, 42]. Because of the localization in momentum space, the probability for reaching high momenta is exponentially suppressed and the atoms stay unionized. This is a purely quantum mechanical effect. Dynamical localization can also happen in the context of quantum dots as predicted by Kravtsov et al [43].

1.5 The Kicked Rotator in higher Dimensions and Experimental Obervations

As established earlier, the Anderson model exhibits localization in one and two dimensions, but a phase transition can occur in higher than two dimensions. This can be seen from the zero of the β function under the one-parameter hypothesis. I will now present a generalization of the kicked rotator and how it can be used to design experiments in atomic condensed matter to establish the theoretical predictions with high accuracy. All these experimental results are taken from the article by Lemarie et al. [44]. The original theory was developed by Fishman et al [45], Casati et al. [46] and Shepelyanski [47].
A simple way of generalizing the kicked rotator is done by adding additional

incommensurate frequencies to the kicking strength so it becomes quasi-periodic

$$H = \frac{p^2}{2} + \lambda(t)\cos\theta \sum_n \delta(t-n) \tag{1.53}$$

$$\lambda(t) = \lambda\left[1 + \epsilon\cos(\omega_2 t + \phi_2)\cos(\omega_3 t + \phi_3)\right]. \tag{1.54}$$

On first sight this seems to have nothing in common with the three dimensional Anderson model. To see that there is a deep connection between these models, one has first to find the correspondence between the quasi-periodic kicked rotator and the three dimensional kicked rotator. Let's start with the 3D kicked rotator

$$H = \frac{p_1^2}{2} + \omega_2 p_2 + \omega_3 p_3 \tag{1.55}$$

$$+\lambda\cos\theta_1\left[1 + \epsilon\cos\theta_2\cos\theta_3\right]\sum_n \delta(t-n) \tag{1.56}$$

and a special initial states

$$\Psi(\theta_1,\theta_2,\theta_3,t=0) \equiv \Xi(\theta_1,t=0)\delta(\theta_2-\phi_2)\delta(\theta_3-\phi_3). \tag{1.57}$$

Because the state is strongly localized in the θ_2 and θ_3 variables, p_2 and p_3 are delocalized completely. In momentum space the state is completely spread in the p_2 and p_3 directions and with a certain distribution in p_1. Again, one can consider the time evolution of one kick with the Floquet operator

$$F\Psi = \mathrm{e}^{i(\lambda\cos\theta_1[1+\epsilon\cos\theta_2\cos\theta_3])} \times \mathrm{e}^{-i\left(p_1^2/2+\omega_2 p_2+\omega_3 p_3\right)}\Psi \tag{1.58}$$

The time evolved state is then in the form

$$\Psi(\theta_1,\theta_2,\theta_3) = \Xi(\theta_1,t)\delta(\theta_2-\phi_2-\omega_2 t)\delta(\theta_3-\phi_3-\omega_3 t) \tag{1.59}$$

$$\Xi(\theta_1,t) = \prod_{t'=1}^{t} \mathrm{e}^{i\left(\lambda\cos\theta_1\left[1+\epsilon\cos(\theta_2+\omega_2 t')\cos(\theta_3+\omega_3 t')\right]\right)}\mathrm{e}^{-ip_1^2/2}\Xi(\theta_1,t=0). \tag{1.60}$$

One can see, that the flat distribution stays the same in momentum space, only the width evolves.

Now one uses the same initial state, but let the time evolution be governed by the quasi-periodic Hamiltonian (1.53). Since it is not periodic in time, the stroboscopic approach doesn't apply anymore. Instead, the wave is acted on by a time evolution operator that changes with time

$$F(t,t-1) = \mathrm{e}^{i(\lambda\cos\theta_1[1+\epsilon\cos(\phi_2+\omega_2 t)\cos(\phi_2+\omega_3 t)])}\mathrm{e}^{-ip_1^2/2}. \tag{1.61}$$

Then the final state at time t is built up from the single step time evolutions

$$\Psi(t) = \prod_{t'=1}^{t} F(t',t'-1)\Psi(t=0). \tag{1.62}$$

Combining this with the plane source state, one can easily see that the $\Xi(\theta_1,t)$ and $\Psi(\theta_1,t)$ evolves just in the same manner as for the 3D kicked rotator, hence for this kind of initial state the Hamiltonians are strictly equivalent. For the

quasi-periodic kicked rotator localization or delocalization happen in the p_1 direction and reflect the properties of a three dimensional kicked system, which in turn is equivalent to the Anderson model in three dimensions. One can see from the time evolution of the state, that the states localized in θ_2, θ_3 move around in time. Since the frequencies are incommensurate, one ensures that all possible phases will be approached with equal probability and an experimental setup would sample all the space. This way the results are not changed by imposing the initial condition of a plane wave onto the state and one effectively simulates an anisotropic 3D Anderson model. A careful observation shows, that with increasing λ the disorder decreases (since the kicking strength affects the hopping, not the disorder). Hence for low λ one can expect localization and for large λ diffusive behaviour. Because the number of possible incommensurate frequencies are not limited, arbitrary dimensions of the Anderson model can be simulated by adding more incommensurate frequencies to the kicking potential.

Such a system can be realized with cold atoms. One can create a periodic potential for atomic condensates by applying a standing wave laser setup (see figure (1.3)).
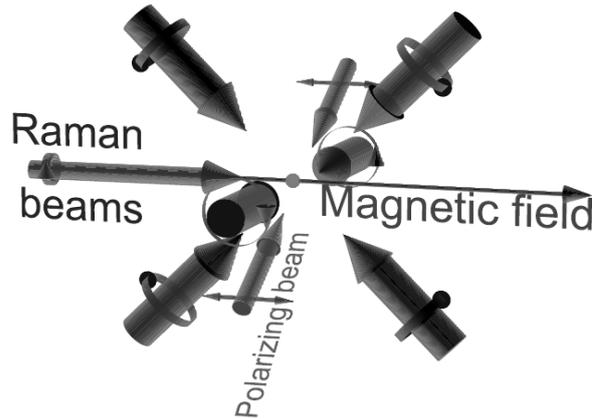
Figure 1.3: A setup to cool down atoms and measure dynamical localization with raman spectroscopy [48].

It should be sufficiently red detuned with respect to the atomic transition such that dissipative effects play no role. If the standing laser is modulated in time and with different frequencies, the Hamiltonian (1.53) describes the system. One starts with a small localized cloud and let it expand for a while, such that the initial conditions are washed out and one basically measures the propagator. The maximum amount of time is limited by the experiment for about 160 kicks. After this is done the momentum components are measured by using doppler shifted absorption of one direction, preferably the direction of fastest dynamics. For the delocalized case one would expect a Gaussian profile in the momentum distribution and for the localized case the typical exponential falloff. The spread in both direction is related to the value of the distribution at $p = 0$ by $\langle p^2 \rangle (t) \sim N^{(-2)}(p = 0)$. So the time development of the spread

can easily tracked by following the development of the $p = 0$ occupation over time without measuring the total momentum profile at each point.
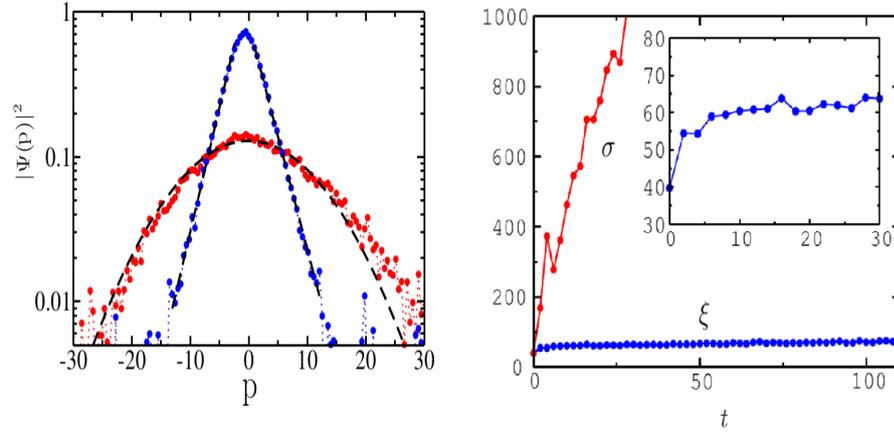
Figure 1.4: The experimentally measured momentum distributions for the localized(blue) and delocalized(red) setup (left figure). The time evolution of $\langle p^2 \rangle$ over time as measured experimentally(right figure).

Indeed, the measurements are in agreement with an exponential decay for the strongly disordered system and a Gaussian spread for the delocalized regime as seen in figure 1.5. Also in the delocalized regime, $\langle p^2 \rangle$ grows linearly in time, as is typical for diffusive behaviour [44]. In the localized regime, $\langle p^2 \rangle$ saturates after a short amount of time.

1.6 Scaling behaviour

Since a real phase transition is expected at the point where the localization sets in, one can define critical exponents. Approaching the critical disorder strength from the insulating side ($\lambda > \lambda_c$), the localization length ξ should diverge with a critical exponent ν as

$$\xi \sim (\lambda - \lambda_c)^{-\nu}. \tag{1.63}$$

However, in the localized regime the spread of the momentum always saturates

$$\left\langle p^2 \right\rangle (t)\big|_{t \to \infty} \sim \xi^2 \sim (\lambda - \lambda_c)^{-2\nu}. \tag{1.64}$$

In the metallic regime ($\lambda < \lambda_c$), the momentum spreads diffusively

$$\left\langle p^2 \right\rangle (t) \sim Dt, \tag{1.65}$$

with a diffusion constant that goes to zero as one approaches criticality

$$D \sim (\lambda_c - \lambda)^s, \tag{1.66}$$

where s is a critical exponent. One could imagine, that at criticality, anomalous diffusion of the form

$$\left\langle p^2 \right\rangle (t) \sim t^k \tag{1.67}$$

with $k \neq 1$ takes place. To find an expression for k, one uses the general scaling hypothesis

$$\left\langle p^2 \right\rangle (t) = t^{k_1} F \left[(\lambda_c - \lambda) t^{k_2} \right], \tag{1.68}$$

where F is an analytical scaling function. To recover the behaviour of the diffusion constant in the metallic limit, $F(x)$ must scale as x^s for large s and one gets

$$\left\langle p^2 \right\rangle (t) = t^{k_1 + sk_2} (\lambda_c - \lambda)^s. \tag{1.69}$$

From this, one can read off that $k_1 + sk_2 = 1$. For large negative x, the scaling function should conform to the insulating behavior, hence $F(x) \sim (-x)^{-2\nu}$, so the time dependence is given by

$$\left\langle p^2 \right\rangle (t) = t^{k_1 - 2\nu k_2} (\lambda_c - \lambda)^{-2\nu}. \tag{1.70}$$

Hence $k_1 - 2\nu k_2 = 0$. One can solve this for k_1 and k_2 and gets

$$k_1 = \frac{2\nu}{s + 2\nu} \tag{1.71}$$

$$k_2 = \frac{1}{s + 2\nu}. \tag{1.72}$$

The piece of information needed to determine the coefficients is Wegners scaling law [49]

$$s = (d - 2)\nu. \tag{1.73}$$

This leads to

$$k_1 = 2/3 \qquad k_2 = 1/3\nu. \tag{1.74}$$

At criticality, where $\lambda_c - \lambda = 0$, the scaling function should be a constant and the universal scaling behaviour of

$$\left\langle p^2 \right\rangle (t) \sim t^{k_1} \sim t^{2/3} \tag{1.75}$$

is predicted. Indeed, experiments are in very good agreement with this (see figure 1.5).
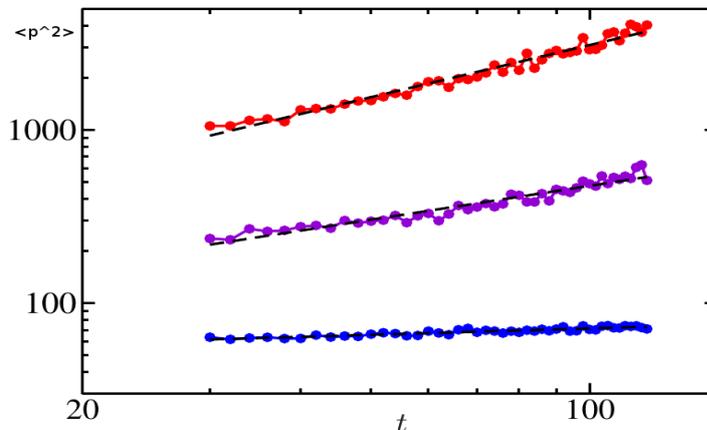
Figure 1.5: Experimentally observed scaling behaviour for the metallic(red), insulating(blue) and anomalous(violet) regime by [44]

1.7   Multifractal behavior

At the Anderson transition, the wave functions of the system change considerably. In the diffusive regime, wave functions are completely delocalized and fill the space uniformly. Suppose a box of size b^d ($b > \lambda$) was put somewhere in the medium. Then the probability of finding the particle $P \sim \int_{b^d} |\psi|^2 \, dr$ is proportional to the size of the box $P \sim b^d$. On the other side of the transition in the strongly localied regime, a box around the center of localization would always contain the whole particle, the scaling of the probability would be independent of the length of the box $P \sim b^0$. In the localized regime the wave function is a pointlike object in space (because it scakes like a point), whereas in the delocalized regime the wave function is d-dimensional. A local dimension dimension can be defined for any measure around any point. The interesting question is, how the transition between d-dimensional and singular object happens. To describe this, one uses the language of multifractality, a concept first developed by Mandelbrot [50] and applied to wave functions by Wegner [51] and Castellani and Peliti [52] .

For a general given measure, in this case $|\psi(r)|^2$, the dimension can be defined locally and typically varies from point to point. The next step is to find a function that measures, how many points have a given dimension. This function is the singularity spectrum. From a mathematical perspective, the singularity spectrum has many similarities with the entropy. Whereas the entropy $S(E)$ is a measure of how many points in probability space have a certain energy E, the singularity spectrum $f(\alpha)$ is a measure of how many points in probability space have the local dimension α. A more rigorous treatment coverering the more mathematical details of dimension, entropy and information can be found in [53]. There are several approaches for the definition of fractal dimensions, but the most common in physics is via the inverse participation ratios (IPR)

$$P_q = \int \left(|\psi(r)|^2 \right)^q d^d r. \tag{1.76}$$

These functions depend on the system size (the case $b = L$) and scale with critical exponents τ_q, that are related to the dimension of the wave function as follows

$$\langle P_q \rangle = L^d \left\langle |\psi|^{2q} \right\rangle \sim L^{-\tau_q}. \tag{1.77}$$

The critical exponents τ_q can then be used to define the fractal dimension D_q

$$D_q = \frac{\tau_q}{q - 1}. \tag{1.78}$$

For the limiting case of the uniform distribution (aka the metal), the fractal dimension is independent of q and equals the space dimension d. In the insulating regime with ideally localized wave packets, the fractal dimension $D_q = 0$. One sees that this definition is in accordance with the intuitive picture for local dimensions developed earlier. However at the critical transition (and around), D_q is indeed a function of q with $0 < D_q < q$.

One can split τ_q in the normal part that scales just like the uniform distribution and the anomalous dimension Δ_q

$$\tau_q = d(q - 1) + \Delta_q. \tag{1.79}$$

This choice for the anomalous dimension is rather convenient. For instance for one wavefunction the spatial correlation of the intensity falls off like Δ_2 [51]

$$L^{2d} \left\langle |\psi^2(r)\psi^2(r')| \right\rangle \sim \left(\frac{|r - r'|}{L} \right)^{\Delta_2}. \tag{1.80}$$

A similar scaling law holds true for the correlations of different wave functions with an energy mismatch ω, where L is substituted by $L_\omega = \left(\frac{\Delta}{\omega} \right)^{1/d}$, Δ is the mean level spacing, as long as $L < L_\omega, \omega > \Delta$ as suggested by Chalker and known as the dynamical scaling hypothesis [54]. Chalker also predicted that the correlations in real and spectral space are related and can be unified to one spatial/spectral correlation function, which was verified in the strong fractal regime [55]

$$C(r, \omega) \sim \left(\frac{|r - r'|}{L_\omega} \right)^{\Delta_2} \qquad (r > l, L_\omega < L), \tag{1.81}$$

l being the mean free path.

The next step is to introduce the singularity spectrum $f(\alpha)$, given formally as the Legendre transform of the exponents τ_q

$$\tau(q) = q\alpha - f(\alpha), \qquad q = \frac{df(\alpha)}{d\alpha}, \qquad \alpha = \frac{d\tau_q}{dq}. \tag{1.82}$$

The singularity spectrum $f(\alpha)$ gives the scaling of all points with local dimension α (here the wave function scales as $|\psi(r)|^2 = L^{-\alpha}$). The number of these points thus scales as $L^{f(\alpha)}$. For a pure metal, $f(\alpha)$ is very sharply peaked at $f(d) = d$ and $f(\alpha) = -\infty$ for all other arguments, which again shows that the definition is meaningful in showing that all points scale the same in a metal. When increasing disorder, this peak becomes first broader and is parabolic (weak multifractality for $d = 2, 2 + \epsilon$), whereas close to criticaly $D_q << d, (d > 3)$

with a non-trivial dependence of the D_q on q. This is known as the strong multifractality.

Mirlin at al. [56] found a symmetry relation between the different anomalous dimensions, namely that

$$\Delta_q = \Delta_{q-1}. \tag{1.83}$$

The anomalous dimensions are thus symmetric around $q = 1/2$, which in turn leads to a relation for the singularity spectrum

$$f(2d - \alpha) = f(\alpha) + d - \alpha. \tag{1.84}$$

Let's look at an experimental verification of those relations. Microwaves are used as opposed to quantummechanical matter waves. There is no problem, since there is a one-to-one correspondence between the stationary Schrödinger equation and the Helmholtz equation. For this reason, many experiments on localization have used classical waves. The experimental challenges are different than for the cold atom experiments. The losses of intensity due to absorption can be quite high and results are sometimes difficult to interpret.
In the following I will describe experiments by Strybulevych et al. [10][57]. They used discs of brazed aluminium beads to simulate a disorded environment (see figure (1.6)).
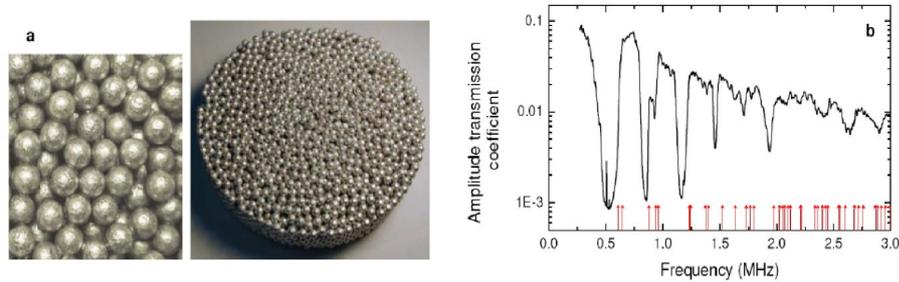
Figure 1.6: a) Left panel: discs of randomly brazed aluminium beads. Right Panel: transmission spectra of these discs. Low transmissions are a hindrance for the experiments. Pictures copied from [10]

One one side of the disc, an ultrasound source is placed to emit waves into the disc. On the opposite side of the disc a probe can measure the intensity of sound waves on the surface. An intensity profile can then be made. The relative disorder strength is controlled via the frequency. The measurements cannot be performed for all frequencies, however there are clearly two frequency bands, one of which has diffusive wave behavior ($\approx 0.2 MHz$) while the other has localized wave packets ($\approx 2.4 MHz$) as seen in figure (1.7).
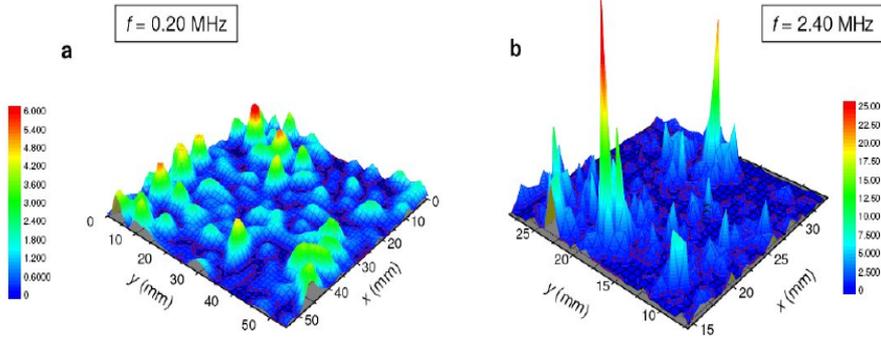
Figure 1.7: Intensity distribution for ultrasound waves propagating through a random medium. a) diffusive regime b) localized regime, pictures are copied from [10]
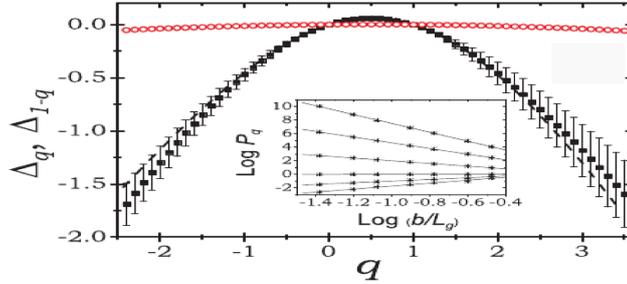
Figure 1.8: Spectrum of the anomalous dimensions (black squares) for the localized ultrasound experiment close to criticality. One can clearly see the symmetry of the curve around $q = 1/2$. The red open circles are for comparison and are measured for diffusive light speckles where $\Delta_q \approx 0$. The inlet shows the bilogarithmic plots for the determination of Δ_q for $q = \{-2, -1, 0, 1, 2, 3\}$ by Strybulevych et al. [57]

Next, the approximate inverse participation ratios were measured. Instead of changing the system size, the coarse graining size b over which the intensity was averaged was varied

$$P_q = \sum_{i=0}^{n} (I_{B_i})^q = \sum_{i=0}^{n} \left[\int_{B_i} I(r) d^d r \right]^q \sim \left(\frac{L}{b} \right)^{-\tau_q} . \qquad (1.85)$$

In this notation, B_i is the ith box, all have the same length b. By varying b, the exponents τ_q and the singularity spectrum $f(\alpha)$ could be determined. By plotting $\ln P_q$ versus $\ln (b/L)$, the anomalous dimensions can be found by the slope of the emerging graphs. The symmetry relation for the Δ_q (1.83) is indeed fulfilled (see figure (1.8)) and it was verified that an anomalous spectrum exists beyond the critical region.

1.8   A short introduction to variable-range hopping transport(VRH)

This introduction is mainly based on a chapter written by Spivak and Shklovskii [66].

It was Mott, who first introduced the concept of VRH [70]. VRH is a process, that is predominant at low temperatures in localized electron systems. One considesr a system with impurity concentration N, the energy levels of which are randomly distributed around a band of width Δ around the Fermi level. The resistance between two impurity centers of such a system is given by

$$\frac{1}{R_{12}} \sim |I(r_{12})|^2 \, \mathrm{e}^{-\frac{\epsilon_{12}}{kT}} \sim \mathrm{e}^{-\frac{2r_{12}}{a}-\frac{\epsilon_{12}}{kT}}. \tag{1.86}$$

Here $I(r_{12})$ is the resonant overlap integral, r_{12} the distance between the centers and a the localization length. The effective energy mismatch between the two impurities is given by

$$\epsilon_{12} = \frac{1}{2}\left(|\epsilon_1 - \epsilon_F| + |\epsilon_2 - \epsilon_F| + |\epsilon_1 - \epsilon_2|\right) \tag{1.87}$$

For a known impurity concentration and width Δ, the typical value of the energy mismatch ϵ_{12} can found to be $\Delta_M = \Delta/Nr_{12}^3$. This result can be used in equation (1.86) to find the distance r_{12} that optimizes the conduction to be

$$r_{12} \approx (T_0/T)^{1/4}, \Delta_M = T_0^{1/4}T^{3/4}, T_0 = \frac{\beta\Delta}{Na^3}, \tag{1.88}$$

where β is a numerical factor.

That origin of an optimal distance can be understood as well. Because the energy levels are randomly distributed, one needs phonons to allow for the inelastic transport of the electrons. However, at low temperatures, phonons are rare and have mostly a small energy. This of course favors hops, with only a small energy mismatch (hence the exponential suppresion in (1.86)). The larger r_{12} is, the more probable a small mismatch of energy is. But, at the same time, the resonant integral decreases, which is another important factor in quantum transport. These two counteracting effects lead to an optimal average hopping distance. Using again equation (1.86) one obtains for the resistivity the following temperature dependence

$$\rho = \rho_0 \mathrm{e}^{\left(\frac{T_0}{T}\right)^{1/4}}. \tag{1.89}$$

How is this effected by Coulomb interactions between the electrons? The Coulomb interaction creates a gap of the single electron density around the Fermi surface [58] . This results in a sligthly different resistivity dependence at low temperatures, because small energy mismatches around the Fermi surface are hindered. This gives for the resistivity the form

$$\rho = \rho_0 \mathrm{e}^{\left(\frac{T_0}{T}\right)^{1/2}}. \tag{1.90}$$

Of importance for this thesis is the question, how interference aspects change the behaviour of the hopping. Because the hopping happens under emission or

absorption of a phonon, phase coherence between hops is lost. But the resonant integral is sensitive to the scattering events during the coherent electron tunneling. Following the rules of quantum mechanics, the overlap integral sums over all ways a particle can tunnel from site 1 to site 2. Since r_{12} is on average larger than the typical distance between the impurities, multiple scatterings have to be taken into account. The remainder of this thesis, will focus on how this overlap integral depends on the occupation of the scattering sites and the nature of the particles.

With these results the introductory part of this thesis is concluded. This however covered merely a fraction of all the mathematical and physical results that have been gathered over the years. The role of interactions, like the dephasing and destruction of single-particle localization at higher temperatures [59] were not discussed. Neither was the interesting topic of Many-Body localization in Fock space [60]. Also the more formal approaches via nonlinear σ-models [61, 62] and the relation with random matrix theories [63, 64] and the classification of symmetric spaces [65] are skipped. However it should be clear, that Anderson localization is an active and still growing field that deserves theoretical and experimental attention.

Most of the results and effects presented here were derived from a single particle picture for which the theory is fairly well understood. The fascinating topic of Anderson localization in an environment with many particles present is less studied and for many questions there is no consensus in the literature. In the following we propose a technique, that can deal with systems if strong local particle-particle interactions are combined with short range hopping at low temperatures in a disordered medium.

Chapter 2

Statement of the problem

In this thesis I want to investigate the localization of particles in a disordered medium when many other particles of the same species are present as well. We want to generalize the known locator expansion originally invented by Abou-Chacra et al. [67]. For a supersymmetric locator expansion see [55, 68].

First a suitable Hamiltonian to model the physical system has to be defined. In this case it will be the Hubbard Hamiltonian, which is local in its interactions and allows only nearest-neighbor hoppings.

2.1   The Hubbard Hamiltonian

The Hubbard Hamiltonian is given by

$$H = \sum_i U_i(\hat{n}_i) - \sum_{\langle i,j \rangle} J_{ij} \left(\hat{b}_j^\dagger \hat{b}_i + \hat{b}_i^\dagger \hat{b}_j \right), \qquad \hat{n}_i = \hat{b}_i^\dagger \hat{b}_i. \tag{2.1}$$

Here the $\hat{b}_i^\dagger$ and $\hat{b}_i$ are the creation and annihilation operators for a particle on site i, the J_{ij} are the tunneling coefficients between neighboring sites. One can see, that the tunneling destroys a particle on one site, but creates another one on a neighboring site. This way, the particle number is conserved.

In the Hubbard approximation [69], only an on-site interaction depending on $\hat{n}_i$ exists. For a finite number of particles, the on-site interaction can always be expanded in a Taylor series.
Suppose one has N particles, then a on-site potential $U_i(\hat{n}_i)$ is defined by the N diagonal elements of the matrix $\langle n_i | U_k(\hat{n}_k) | n_j \rangle = U(n_i)\delta_{n_i,n_j}$.

Hence

$$U_i(n) = \sum_{j=0}^N U_i^j n^j. \tag{2.2}$$

This can be rewritten as a $(N+1) \times (N+1)$ matrix equation

$$
\begin{pmatrix} U_i(0) \\ \vdots \\ U_i(N) \end{pmatrix} = \begin{pmatrix} 0^0 & 0^1 & 0^2 & \cdots & 0^N \\ 1^0 & 1^1 & 1^2 & \cdots & 1^N \\ \vdots & \vdots & \ddots & & \vdots \\ \vdots & \vdots & & \ddots & \vdots \\ N^0 & N^1 & N^2 & \cdots & N^N \end{pmatrix} \begin{pmatrix} U_i^0 \\ \vdots \\ U_i^N \end{pmatrix} \tag{2.3}
$$

Since all the rows of the matrix are linearly independent, it is an invertible matrix and one can always find the Taylor coefficients.

For physical applications one can assume, that $U_i(0) = const$ troughout the system. Also, since the interactions do not depend on the depth of the well the particle is in, one can conjecture that $U_i(n) - U_i(1)$ is a function of $n > 1$, that is independent of the lattice site i. For a disordered lattice, intuitively one would expect $U_i(1)$ to vary from crystal site to crystal site according to a probability distribution $\rho(U_i(1))$. The J_{ij} can be assumed to be constant for all nearest neighbor pairs (i,j). A magnetic field would give an additional phase factor to each connection between two sites. The number of nearest neighbors depends on the lattice geometry and the dimension d of the system.

For fermions and hard-core bosons, only the occupation numbers $0, 1$ are of importance. One can use the Heisenberg equation of motion to find the time dependence of an annihilation operator. By taking $U_i(0) = 0$ everywhere on the lattice and in the absence of a magnetic field, one has in the non-interacting case

$$
H = \sum_i \epsilon_i n_i - \sum_{\langle ij \rangle} J \left(\hat{b}_j^\dagger \hat{b}_i + \hat{b}_i^\dagger \hat{b}_j \right). \tag{2.4}
$$

This Hamiltonian can be used to create the time evolution of the creation/annihilation operators via the Heisenberg equation of motion

$$
i\dot{\hat{b}}_i(t) = \left[\hat{b}_i(t), H \right]. \tag{2.5}
$$

2.2   Hard-core Bosons and their commutation relation

One of the purposes of this thesis is to verify the prediction Müller made about the Green's functions of fermions and hard-core bosons . He argues that despite very similar level occupations, the Green's functions do differ by signs [75]

$$
\frac{G_{i,0}^R(\omega)}{G_{0,0}^R(\omega)} = \sum_{P=\{j_0=0,\ldots,j_l=i\}} \prod_1^l \frac{J \left[\mathrm{sgn}(\epsilon_{j_p}) \right]^B}{\epsilon_{j_p} - \omega} \tag{2.6}
$$

This equation describes how the Green's function behaves by summing over the contributions of all possible paths P between the site 0 and i and their factors which depend on the random on-site energies ϵ_i and on the nature of the particles, $B = 0$ for fermions and $B = 1$ for hard-core bosons. The equation was derived by the truncation of the Hilbert space for hard-core bosons and by

assuming the commutation law $\left[\hat{b}_i^\dagger, \hat{b}_j\right]_B = \delta_{ij}\left[1 - 2B\left(1 - \hat{n}_i\right)\right]$. This however has to be taken with care, because this relation technically holds not for all hard-core bosons.

In nature there are in principle two distinct types of hard-core bosons.
The first kind is of composite nature, as in Cooper pairs [72]. Here the boson is built up from two fermions

$$\hat{b}^\dagger = \hat{c}_\uparrow^\dagger \hat{c}_\downarrow^\dagger. \tag{2.7}$$

Since fermionic operators fulfill the identity $\hat{c}^\dagger \hat{c}^\dagger = \hat{c}\hat{c} = 0$, for this kind of hard-core bosons the relation

$$\hat{b}^\dagger \hat{b}^\dagger = 0, \tag{2.8}$$

strictly holds. Further then

$$\left[\hat{b}, \hat{b}^\dagger\right] = 1 - 2\hat{b}^\dagger \hat{b}. \tag{2.9}$$

Then there is the case of strongly interacting hard-core bosons. This means, that they can never occupy the same state, because of an energetic penalty. Nonetheless, regular bosons (even with interactions) can create two particles in a state $\hat{b}^\dagger \hat{b}^\dagger |0\rangle = |2\rangle$.
I want to find an algebra, that effectively describes hard-core bosons. Given a bosonic system, one starts with a set of bosonic creation operators $\hat{b}_i^\dagger$, where i denotes the lattice site. The application of those creation operators on the vacuum create Fock-states at each site. It is enough to focus on one lattice site and remove the index i. For convenience, a finite Fock space is assumed, i.e. $|0\rangle, |1\rangle, \cdots |N\rangle$. Then the hard-core boson creation operator $\hat{a}^\dagger$ should be a linear combination of all the other creation operators $\hat{a}^\dagger = \sum_{i=0}^N a_i \left(\hat{b}^\dagger\right)^i$. The bosons should depend on some parameter U (it is dimensionless and in this section not an interaction energy!) that describes, how strong the repulsions are. The case of hard-core bosons is the limit of $U \to \infty$.
One also demands that

$$\langle 0|a\rangle = 0 \tag{2.10}$$

$$\langle 1|a\rangle = 1 - O(\frac{1}{U}) \tag{2.11}$$

$$\langle n|a\rangle = O(\frac{1}{U}) \tag{2.12}$$

This means, by increasing the repulsion, it should be less and less likely to find a particle in a state with a higher occupation number than one. One possible normalized creation operator looks like this

$$\hat{a}^\dagger = C \left(\sum_{j=1}^N \frac{\mathrm{e}^{-U(j-1)/2}\left(\hat{b}^\dagger\right)^j}{\sqrt{j!}}\right), C = \sqrt{\frac{1 - \mathrm{e}^{-U}}{1 - \mathrm{e}^{-U(N-1)}}} \tag{2.13}$$

Taking the commutator of that expression gives

$$\left[\hat{a}, \hat{a}^\dagger\right] = |C|^2 \sum_{j=1}^{N} \sum_{k=1}^{N} \frac{\mathrm{e}^{-\frac{U}{2}(j+k-2)}}{\sqrt{j!}\sqrt{k!}} \left[\hat{b}^j, (\hat{b}^\dagger)^k\right] \tag{2.14}$$

$$= |C|^2 \left(\left[\hat{b}, \hat{b}^\dagger\right] + \mathrm{e}^{-\frac{U}{2}}\left[\cdots\right]\right). \tag{2.15}$$

The term in parentheses in the second term on the right hand side is decreasing with U and has an upper bound. Hence in the limit of hard-core bosons

$$\lim_{U \to \infty} \left[\hat{a}, \hat{a}^\dagger\right] = 1. \tag{2.16}$$

So mathematically, there is a difference between these two types of bosons even in the limit of infinitively repulsive interactions. However, one could never directly observe this difference.

The purpose of this thesis is to introduce a technique that does not only allow to calculate the Green's function for hard-core bosons without a truncation of Hilbert space and alteration of commuation laws, but is also capable of producing corrections when the interactions are not infinitely strong. As will be shown with the help of Hubbard operators, the single particle Green's functions obtain corrections of the order $(W/U)^{-1}$, W being the bandwidth of the energy distribution and U the interaction potential.

2.3 The failure of the equation of motion approach

In this section it will be shown, that the classical approach via normal via equations of motion leads to equations that cannot be handled at all. Especially it will be obvious that there is no good parameter one can use to develop a theory for hard-core bosons $U \to \infty$.

The usual particle creation and annihilation operators are given by $\hat{c}^\dagger$ and $\hat{c}$, which fulfill the commutation/anticommutation relation

$$\left[\hat{c}_i, \hat{c}_j^\dagger\right]_\eta = \delta_{ij}, \qquad [A, B]_\eta = AB - \eta BA \tag{2.17}$$

where $\eta = \pm 1$. The $+$ is for bosons, the $-$ is for fermions. The Green's function is defined as

$$G_{AB}^\pm(t, t') = \mp \mathrm{i}\Theta\{\pm(t - t')\} \left\langle [A(t), B(t')]_\eta \right\rangle, \tag{2.18}$$

and the thermal quantum mechanical average as

$$\langle X \rangle = Z^{-1} \mathrm{Tr}\left\{X \mathrm{e}^{-\beta(H-\mu N)}\right\}, \qquad Z = \mathrm{Tr}\left\{\mathrm{e}^{-\beta(H-\mu N)}\right\}. \tag{2.19}$$

The time-dependent operators are given in the Heisenberg picture by

$$A(t) = \mathrm{e}^{\mathrm{i}Ht} A(0) \mathrm{e}^{-\mathrm{i}Ht} \tag{2.20}$$

The Green's function satisfy the equation of motion

$$\mathrm{i}\frac{d}{dt}G^{\pm}_{AB}(t,t') = \delta(t-t')\left\langle [A(t),B(t')]_\eta \right\rangle + G^{\pm}_{[A,H],B}(t,t') \tag{2.21}$$

One can define the Fourier transform as

$$G^{\pm}_{A,B}(\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty}G^{\pm}_{A,B}(t)\mathrm{e}^{\mathrm{i}\omega t}dt. \tag{2.22}$$

This function can be generalized for complex ω which is everywhere defined but on the real axis

$$G_{A,B}(\omega) = G^{+}_{A,B}(\omega) \text{ if } \Im\omega > 0, \tag{2.23}$$

$$G^{-}_{A,B}(\omega) \text{ if } \Im E < 0. \tag{2.24}$$

A Fourier transform of the equation of motion (2.21) shows that

$$\omega G_{A,B}(\omega) = \frac{1}{2\pi}\left\langle [A,B] \right\rangle + G_{[A,H],B}(\omega) \tag{2.25}$$

and it can be further shown that

$$\langle B(t')A(t)\rangle = \mathrm{i}\lim_{\epsilon\to 0^+}\int_{-\infty}^{\infty}\left[G_{A,B}(\omega+\mathrm{i}\epsilon) - G_{A,B}(\omega-\mathrm{i}\epsilon)\right]\frac{\mathrm{e}^{-\mathrm{i}\omega(t-t')}}{\mathrm{e}^{\beta(\omega-\mu)}-\eta}d\omega. \tag{2.26}$$

For both fermions and bosons one has

$$\left[\hat{b}_i,\hat{n}_j\right] = \delta_{ij}\hat{b}_j \tag{2.27}$$

2.4 Approximation for the atomic limit

In the atomic limit (no tunneling between sites, no disorder) one has as a Hamiltonian for bosons approximately

$$H = T_0\sum_i n_i + \frac{1}{2}U\sum_i \hat{n}_i\left(\hat{n}_i - 1\right), \tag{2.28}$$

given of course, that the repulsion is very strong and one has a simplified interaction (one particle reacts with all others on that site equivalently, no spins). This is of course equivalent to

$$H = \left(T_0 - \frac{U}{2}\right)\sum_i \hat{n}_i + \frac{U}{2}\sum_i \hat{n}_i^2. \tag{2.29}$$

Certainly, making the hardcore boson assumption $\hat{n}_i^2 = \hat{n}_i$ at the beginning, one receives immediately the single particle Hamiltonian $H = T_0\sum_i \hat{n}_i$ But withstanding the temptation for this simplification for now leads then to

$$\mathrm{i}\dot{\hat{b}}_i(t) = \left[\hat{b}_i(t),H\right] = \left(T_0 + U\right)\hat{b}_i(t) + U\hat{n}_i\hat{b}_i(t) \tag{2.30}$$

This in return means that

$$\mathrm{i}\frac{d}{dt}G^{+}_{ij}(t-t') = \delta(t-t') + \left(T_0 + \frac{U}{2}\right)G^{+}_{ij} + \frac{U}{2}\Gamma^{1+}_{ij}(t-t') \tag{2.31}$$

Here $\Gamma_{ij}^{1+} = -\mathrm{i}\Theta(t-t')\left\langle \left[\hat{n}_i \hat{b}_i(t), \hat{b}_j^\dagger(t')\right]\right\rangle$. One can then find the equation of motion for Γ as well

$$\mathrm{i}\frac{d}{dt}\Gamma_{ij}^{1+}(t-t') = \delta(t-t')\left\langle \left[\hat{n}_i \hat{b}_i(0), \hat{b}_j^\dagger(0)\right]\right\rangle - \mathrm{i}\Theta(t-t')\left\langle \left[i\left(\dot{\hat{n}_i \hat{b}_i}\right)(t), \hat{b}_j^\dagger(t')\right]\right\rangle \tag{2.32}$$

One has that $\left\langle \left[\hat{n}_i \hat{b}_i(0), \hat{b}_j^\dagger(0)\right]\right\rangle = 2\delta_{ij}\left\langle \hat{n}_i\right\rangle$. Using the basic commutators, one has $\left[\hat{n}_i \hat{b}_i, \hat{n}_j\right] = \delta_{ij}\hat{n}_i$. Also one has that $\left[\hat{n}_i \hat{b}_i, \hat{n}_j\right] = \delta_{ij}\left(2\hat{n}_i^2 \hat{b}_i + \hat{n}_i \hat{b}_i\right)$. This leaves us with

$$\mathrm{i}\frac{d}{dt}\Gamma_{ij}^{1+}(t-t') = \delta(t-t')2\left\langle \hat{n}_i\right\rangle + T_0 \Gamma_{ij}^{1+}(t-t') + U\Gamma_{ij}^{2+}(t-t'), \tag{2.33}$$

with $\Gamma_{ij}^{2+}(t-t') = -\mathrm{i}\Theta(t-t')\left\langle \left[\hat{n}_i^2 \hat{b}_i(t), \hat{b}_j^\dagger(t')\right]\right\rangle$.

The two final equations can also be conveniently written as Fourier transforms (retarded and advanced)

$$E G_{ij}(\omega) = \frac{1}{2\pi}\delta_{ij} + \left(T_0 + \frac{U}{2}\right)G_{ij}(\omega) + \frac{U}{2}\Gamma_{ij}^1(\omega) \tag{2.34}$$

$$\omega\Gamma_{ij}^1(\omega) = \frac{1}{2\pi}\delta_{ij}2\left\langle \hat{n}_i\right\rangle + T_0 \Gamma_{ij}^1(\omega) + U\Gamma_{ij}^2(\omega) \tag{2.35}$$

One could go further towards finding $\Gamma_{ij}^2(\omega)$ which would require $\Gamma_{ij}^3(\omega)$. This of course goes on recursively. After setting $\Gamma^2 = 0$, one finds for $\Gamma_{ij}^1(\omega)$

$$\Gamma_{ij}^1(\omega) = \frac{\delta_{ij}\left\langle \hat{n}_i\right\rangle}{\pi\left(\omega - (T_0 + U)\right)}. \tag{2.36}$$

Thus

$$\Gamma_{ij}(\omega) = \frac{\delta_{ij}}{2\pi}\left(\frac{1 - 2\left\langle \hat{n}_i\right\rangle}{\omega - \left(T_0 + \frac{U}{2}\right)} + \frac{2\left\langle \hat{n}_i\right\rangle}{\omega - (T_0 + U)}\right). \tag{2.37}$$

This means, one has a splitting into two energy bands. The choice of where to make the approximation did change the result seemingly qualitatively. However, one should remind oneself, that the second energy band should be never occupied in the hard-core approximation, so the two results are physically the same.

2.5　Inclusion of tunneling

Starting point is the equation of motion

$$\mathrm{i}\frac{d}{dt}G_{i,j}^R = \delta(t-t')\delta_{ij} - \mathrm{i}\Theta(t-t')\left\langle \left[\left[\hat{b}_i(t), H\right], \hat{b}^\dagger(t')\right]\right\rangle. \tag{2.38}$$

Using the Hubbard-Hamiltonian with interactions

$$H = \sum_i \epsilon_i \hat{n}_i - J\sum_{ij}\left(\hat{b}_i^\dagger \hat{b}_j + \hat{b}_i^\dagger \hat{b}_j\right) + \frac{U}{2}\sum_i \hat{n}_i\left(\hat{n}_i - 1\right). \tag{2.39}$$

For the treatment of the equation of motion, the following identities are very useful

$$\left[\hat{b}_i, \hat{n}_j\right] = \delta_{ij}\hat{b}_j; \quad \left[\hat{b}_i, \hat{b}_j^\dagger\hat{b}_k + \hat{b}_k^\dagger\hat{b}_j\right] = \delta_{ij}\hat{b}_k + \delta_{ki}\hat{b}_j \qquad (2.40)$$

$$\left[\hat{n}_i\hat{b}_i, \hat{n}_j\right] = \delta_{ij}\hat{n}_i; \quad \left[\hat{n}_i\hat{b}_i, \hat{n}_j\right] = \delta_{ij}\left(2\hat{n}_i^2\hat{b}_i + \hat{n}_i\hat{b}_i\right). \qquad (2.41)$$

It is convenient to rewrite the Hamiltonian in terms of $\tilde{\epsilon}_i = \epsilon_i - U$, $\tilde{U} = \frac{U}{2}$. The tildes are ommited further on.

$$H = \sum_i \epsilon_i\hat{n}_i - J\sum_{ij}\left(\hat{b}_i^\dagger\hat{b}_j + \hat{b}_i^\dagger\hat{b}_j\right) + U\sum_i \hat{n}_i^2 \qquad (2.42)$$

In the following I will build up a hierarchy of Green's functions. Since the Hamiltonian is time independent, it is convenient to work with the Fourier-transformed $F(f)(\omega) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^\infty f(t)\mathrm{e}^{-\mathrm{i}\omega t}\,dt$ equations

$$-\omega G_{ij}(\omega) = \frac{\delta_{ij}}{\sqrt{2\pi}} + G_{\left[\hat{b}_i, H\right], \hat{b}_j^\dagger}(\omega) \qquad (2.43)$$

$$= \frac{\delta_{ij}}{\sqrt{2\pi}} + (\epsilon_i + U)G_{ij}(\omega) - J\sum_{k\in\partial_i} G_{kj}(\omega) + 2G_{\hat{n}_i\hat{b}_i, \hat{b}_j^\dagger}(\omega) \qquad (2.44)$$

Let's again define

$$\Gamma_{ij}^n(\omega) = G_{\hat{n}_i^n\hat{b}_i, \hat{b}_j^\dagger}(\omega). \qquad (2.45)$$

Then one has the time derivative

$$\mathrm{i}\frac{d}{dt}\Gamma_{ij}^m = \delta(t - t')\delta_{ij}\left\langle\left[\hat{n}^m\hat{b}, \hat{b}^\dagger\right]\right\rangle - \mathrm{i}\Theta\left\langle\left[i\left(\dot{\hat{n}_i^m\hat{b}_i}\right)\hat{b}_j^\dagger\right]\right\rangle \qquad (2.46)$$

The very first average equals (see the appendix for advanced commutator relations)

$$\left\langle\left[\hat{n}^m\hat{b}, \hat{b}^\dagger\right]\right\rangle = \left\langle\hat{n}^m + \sum_{k=0}^{m-1}(-1)^k C_{mk}\hat{n}^{m-k}\right\rangle, \quad C_{mk} = \sum_{s=0}^{m-1-k}\binom{s+k}{s} \qquad (2.47)$$

Now

$$\mathrm{i}\left(\dot{\hat{n}_i^m\hat{b}_i}\right) = \left[\hat{n}_i^m\hat{b}_i, H\right] \qquad (2.48)$$

Here one needs to evaluate the commutator of that Hamiltonian step by step

$$\left[\hat{n}_i^m\hat{b}_i, \sum_k \epsilon_k\hat{n}_k\right] = \epsilon_i\hat{n}_i^m\hat{b}_i \qquad (2.49)$$

Then also

$$\left[\hat{n}_i^m\hat{b}_i, -J\sum_{\langle jk\rangle}\left(\hat{b}_j^\dagger\hat{b}_k + \hat{b}_k^\dagger\hat{b}_j\right)\right] = -2J\sum_{\langle jk\rangle}\left[\hat{n}_i^m\hat{b}_i, \hat{b}_j^\dagger\hat{b}_k\right] \qquad (2.50)$$

$$= -2J\sum_{j\in\delta_i}\left(\hat{n}_i^m\hat{b}_j + \sum_{s=0}^{m-1}(-1)^s C_{ms}\hat{n}_i^{m-s}\hat{b}_j - \hat{b}_j^\dagger\left(\sum_{s=0}^{m-1}C_{ms}\hat{n}_i^{m-1-s}\right)\hat{b}_i^2\right) \qquad (2.51)$$

Lastly

$$\left[\hat{n}_i^m \hat{b}_i, U\sum_k \hat{n}_k^2\right] = U\left(2\hat{n}_i^{m+1}\hat{b}_i + \hat{n}_i^m \hat{b}_i\right) \tag{2.52}$$

Defining

$$\Xi_{ikj}^m = G_{\hat{n}_i^m \hat{b}_k, \hat{b}_j^\dagger}, \tag{2.53}$$

one comes to the conclusion, that the equation of motion for the Γ^m is

$$-\omega\Gamma_{ij}^m = \frac{\delta_{ij}}{\sqrt{2\pi}}\left\langle \hat{n}^m + \sum_{k=0}^{m-1}(-1)^k C_{mk}\hat{n}^{m-k}\right\rangle + \epsilon_i\Gamma_{ij}^m \tag{2.54}$$

$$- 2J\sum_{k\in\partial_i}\left(\Xi_{ikj}^m + \sum_{s=0}^{m-1}(-1)^s C_{ms}\Xi_{ikj}^{m-s} - \sum_{s=0}^{m-1}C_{ms}G_{\hat{n}_i^{m-1-s}\hat{b}_k^\dagger \hat{b}_i^2, \hat{b}_j^\dagger}\right) + U\left(2\Gamma_{ij}^{m+1} + \Gamma_{ij}^m\right)$$
$$\tag{2.55}$$

Here it becomes apparent, why this approach is not very convenient. For once, one creates a big and clumsy hierarchy of equations. It is hard to judge, at which point a truncation would be meaningful, since there is no small parameter for expansion. Even more disturbing is the presence of the interaction strength U in those equations, since one is interested in the limit of $U \to \infty$. For those reasons, Hubbard operators will be introduced.

Chapter 3

Hubbard operators and their basic properties

The idea of Hubbard operators is not exactly new, but its application to bosonic system really only became necessary after the advent of experimental cold-atom techniques. The Hubbard operators were first introduced by Hubbard in 1967 [71] and applied to describe phenomena in fermionic systems.

For a single site the Hubbard operator connects two states $X_{ij} = |n_i\rangle \langle n_j|$. One has that $X^{ij}X^{kl} = \delta_{jk}X^{il}$. From this then follows

$$[X_{ij}, X_{kl}] = |n_i\rangle \langle n_j| |n_k\rangle \langle n_l| - |n_k\rangle \langle n_l| |n_i\rangle \langle n_j| = \delta_{jk}X_{il} - \delta_{li}X_{kj} \qquad (3.1)$$

For different lattice sites t and s this generalizes to

$$\left[X_{ij}^{(s)}, X_{kl}^{(t)}\right] = \delta_{st}\left(\delta_{jk}X_{il} - \delta_{li}X_{kj}\right) \qquad (3.2)$$

The anti commutator is then given by

$$\{X_{ij}, X_{kl}\} = \delta_{jk}X_{il} + \delta_{li}X_{kj} \qquad (3.3)$$

The difference to the fermionic case lies in the allowed values of i, j, k and l. One needs the correspondence between the regular creation and annihilation operators and the Hubbard operators. One has to demand that $\langle n| \hat{n} |n\rangle = n$ for all the allowed values of n and that the typical commutation relations are obeyed

$$\left[\hat{a}_i, \hat{a}_j^\dagger\right]_\mp = \delta_{ij}. \qquad (3.4)$$

For spinless fermions this can only be

$$\hat{c}^\dagger = X^{10}, \qquad \hat{c} = X^{01} \qquad (3.5)$$

whereas for bosons one must have (up to an overall phase factor)

$$\hat{b}^\dagger = \sum_{n=0}^{\infty} \sqrt{n+1}X^{n+1,n}, \qquad \hat{b} = \sum_{n=0}^{\infty} \sqrt{n+1}X^{n,n+1} \qquad (3.6)$$

Then

$$\hat{b}^\dagger \hat{b} = \sum_{n,n'=0}^{\infty} \sqrt{n+1}\sqrt{n'+1} X^{n+1,n} X^{n'1,n'+1} \tag{3.7}$$

$$= \sum_{n,n'=0}^{\infty} \sqrt{n+1}\sqrt{n'+1} X^{n+1,n'+1} \delta_{n,n'} = \sum_{n=0}^{\infty}(n+1)X^{n+1,n+1} = \hat{n}. \tag{3.8}$$

Also one can check that

$$\left[\hat{b}, \hat{b}^\dagger\right]_- = \hat{b}\hat{b}^\dagger - \hat{b}^\dagger\hat{b} = \sum_{n=0}^{\infty}(n+1)X^{n,n} - \sum_{n=1}^{\infty}(n)X^{n,n} = \sum_{n=0}^{\infty}X^{n,n} = I. \tag{3.9}$$

One wants to use (3.7) on the general Hubbard Hamiltonian (2.39). Now the basis for the Hubbard operators are the Fock states of the different lattice sites $|n_i\rangle$. The one-site Hubbard operators themselves are of the form $X_i^{n_1,n_2} = |n_1\rangle\langle n_2|_i$. They are tensor products of Hubbard operators of all sites, but the other sides are represented by the identity. Since the product states for a complete set, all the operators can be represented by Hubbard states. The Bose-Hubbard hamiltonian can then be rewritten as

$$H = \sum_i \sum_{n_i} \epsilon_i n_i |n_i\rangle\langle n_i| + J\sum_{\langle i,j\rangle} \sum_{n_i=0,n_j 1} \left(\sqrt{(n_i+1)\,n_j}\,|n_i+1\rangle\langle n_i||n_j-1\rangle\langle n_j|\right. \tag{3.10}$$

$$\left. + \sqrt{n_i\,(n_j+1)}\,|n_i-1\rangle\langle n_i||n_j+1\rangle\langle n_j|\right) + U\sum_i \sum_{n_i} n_i\,(n_i-1)\,|n_i\rangle\langle n_i|. \tag{3.11}$$

Without hopping, the Hubbard operators diagonalize the single site Hamiltonian

$$U = \sum_{n_i}\left(\epsilon_i n_i + U n_i\,(n_i-1)\right)X^{n_i,n_i} \tag{3.12}$$

A toy model of a hard core system with only one excitable mode per site without hopping would look like

$$H^0 = \sum_i \epsilon_i X_i^{11} + \sum_j (2\epsilon_j + 2U)\,X_j^{22}. \tag{3.13}$$

One can also use the Hubbard operators to find a new representation for the thermal one-particle Green's function

$$G_{kl}(\tau_1 - \tau_2) \equiv \left\langle T_\tau \hat{b}_k(\tau_1)\hat{b}_l^\dagger(\tau_2)\right\rangle = \sum_{i,j=0}^{\infty} \sqrt{i+1}\sqrt{j+1}\left\langle T_\tau \tilde{X}_k^{i,i+1}(\tau_1)\tilde{X}_l^{j+1,j}(\tau_2)\right\rangle. \tag{3.14}$$

As start for the perturbation one always uses

$$\left\langle T_\tau \tilde{X}_k^{ij}(\tau_1)\tilde{X}_l^{ji}(\tau_2)\right\rangle = \frac{\left\langle T_\tau X_k^{i,i+1}(\tau_1)X^{j+1,j}\sigma(\beta)\right\rangle_0}{\left\langle\sigma(\beta)\right\rangle_0} \tag{3.15}$$

For the general setup one demands that $\lambda_k^p = (\epsilon_k p + U p\,(p-1))$. With $p, q = 0, 1$ for fermions and $p, q \in \mathbb{Z}_+$ for bosons. H_{int} is given by

$$H_{int} = J \sum_{r,s=0}^{\infty} \sqrt{r+1}\sqrt{s+1} \left(X_1^{r+1,r} X_2^{s,s+1} + X_2^{r+1,r} X_1^{s,s+1} \right). \qquad (3.16)$$

For the evaluation of the Green's function, one needs to expand the $\sigma(\beta)$ matrix

$$\sigma(\beta) = T_\tau \mathrm{e}^{-\int_0^\beta H_{int}(\tau)d\tau} = T_\tau \left(1 - \int_0^\beta H_{int}(\tau)d\tau + \frac{1}{2} \int_0^\beta \int_0^\beta H_{int}(\tau_1)(\tau_2)d\tau_1\,d\tau_2 \dots \right)$$
$$(3.17)$$

What follows are averages of products of Hubbard operators, that have to be handled with care.

3.1 Wick's Theorem

For almost all applications in Many-body physics, one is interested in the time-ordered quantum thermodynamical average of a product of operators with respect to the original Hamiltonian

$$\left\langle T \prod_i X^i \right\rangle = \frac{1}{Z} \mathrm{Tr} \left(T \mathrm{e}^{-\beta H_0} \prod_i X^i \right), \qquad Z = \mathrm{Tr}\, \mathrm{e}^{-\beta H_0}. \qquad (3.18)$$

Because the operators do not commute, the normal form of Wick's theorem doesn't apply anymore. Instead one has to use a general form that I found without proof in a paper by Slobodyan[74].

$$\left\langle T\{X_1^{\alpha_1} \dots X_{m-1}^{\alpha_{m-1}}(\tau_{m-1}) X_0^\alpha(\tau) X_{m+1}^{\alpha_{m+1}}(\tau_{m+1}) \dots X_n^{\alpha_n}(\tau_n)\} \right\rangle_0 \qquad (3.19)$$

$$= (-1)^{p_1} g_{01}^\alpha(\tau - \tau_1) \left\langle T\{[X_1^{\alpha_1}, X_1^\alpha]_{\mp}^{\tau_1} X_2^{\alpha_2}(\tau_2) \dots X_n^{\alpha_n}(\tau_n)\} \right\rangle_0 + \dots \qquad (3.20)$$

$$\dots (-1)^{p_n} g_{0n}^\alpha(\tau - \tau_n) \left\langle T\{X_1^{\alpha_1}(\tau_1) \dots X_{n-1}^{\alpha_{n-1}}(\tau_{n-1}) [X_n^{\alpha_n}, X_n^\alpha]_{\mp}^{\tau_n}\} \right\rangle_0, \qquad (3.21)$$

where p_i is the number of Fermi transpositions of the operator $X_0^\alpha(\tau)$ from the original position to the position $\dots X_i^{\alpha_i}(\tau_i) X_0^\alpha(\tau) \dots$ plus 1. For bosonic operators $p_i = 0$. The $g_{0i}^\alpha(\tau - \tau_i)$ are the Green's functions of the "zeroth approximation" :

$$g_{0i}^\alpha(\tau - \tau_i) = \delta_{0i} g^\alpha(\tau - \tau_i) \qquad (3.22)$$

$$(3.23)$$

Using the linearity in the Hamiltonian, one gets

$$g^{pq}(\tau - \tau_i) = \mathrm{e}^{(\tau - \tau_i)\lambda_{pq}} \left\{ \begin{array}{l} n^{\mp}(\lambda_{pq}), \tau > \tau_i \\ n^{\mp}(\lambda_{pq}) \pm 1, \tau < \tau_i \end{array} \right. \qquad (3.24)$$

with

$$n^{\pm}(\lambda_\alpha) = \left(\mathrm{e}^{\beta\lambda_\alpha} \mp 1 \right)^{-1}. \qquad (3.25)$$

The upper sign is always for bosons, the lower for fermions. Probably more important is the frequency representation of g^{pq}, which is given by

$$g^{pq}(\omega_n) = \frac{\mp 1}{\beta\,(\mathrm{i}\omega_n - \lambda_{pq})} - \qquad (3.26)$$

The proof of the generalized form of Wick's theorem follows basically the one for the regular Wick's theorem in the book by Bruus and Flensberg [73] and uses the equation of motion technique. The Green's function for $n/2$ particle non-diagonal Hubbard operators is defined as

$$G_0^{(n)}(\alpha_1\tau_1, \cdots \alpha_n\tau_n) = (-1)^n \left\langle T_\tau \left[X^{\alpha_1}(\tau_1) \ldots X^{\alpha_n}(\tau_n) \right] \right\rangle. \tag{3.27}$$

Note that n must be even for the Green's function not to vanish.
The permutation of n operators is defined as

$$P(X^{\alpha_1}(\tau_1) \ldots X^{\alpha_2}(\tau_n)) = X^{\alpha_{P1}}(\tau_{P1}) \ldots X^{\alpha_{Pn}}(\tau_{Pn}), \tag{3.28}$$

where Pj is the jth variable of the permutation P. If one takes the bosonic or fermionic nature of the Hubbard operators for granted, then the time ordering prescription is unambigious and one can rewrite the definition as

$$G_0^n(\alpha_1, \ldots, \alpha_2) = (-1)^n \sum_{P \in S_n} (\pm)^P \Theta(\tau_{P1} - \tau_{P_2}) \cdots \Theta(\tau_{P(n-1)} - \tau_{P_n}) \left\langle X^{\alpha_{P1}}(\tau_{P1}) \ldots X^{\alpha_{Pn}}(\tau_{Pn}) \right\rangle. \tag{3.29}$$

The Θs are just the regular Heaviside functions. If one takes the derivative with respect to any τ_1 of the above equation, one gets two contributions, one by the derivative of the Θ function, the other by the derivative of the time dependent operators. Using the equation of motion technique, one can show that in the case for two operators

$$-\partial_{\tau_1} G^1_{\alpha_1\alpha_2}(\tau_1 - \tau_2) = \frac{\partial}{\partial \tau_1} \left(\Theta(\tau_1 - \tau_2) \left\langle X^{\alpha_1}(\tau_1) X^{\alpha_2}(\tau_2) \right\rangle \pm \Theta(\tau_2 - \tau_1) \left\langle X^{\alpha_2}(\tau_2) X^{\alpha_1}(\tau_1) \right\rangle \right) \tag{3.30}$$

$$= \delta(\tau_1 - \tau_2) \left\langle [X^{\alpha_1}, X^{\alpha_2}]_\mp (\tau_2) \right\rangle + \left\langle T_\tau \left([H_0, X^{\alpha_1}](\tau_1) X^{\alpha_2}(\tau_2) \right) \right\rangle \tag{3.31}$$

For the free case one has $H_0 = \sum_i \lambda_i X^{ii}$. So $[H_0, X^\alpha] = \lambda_\alpha X^\alpha$ with $\lambda_{pq} = \lambda_p - \lambda_q$. Then it follows that

$$\frac{-\partial_{\tau_1} - \lambda_{pq}}{\left\langle [X^{\alpha_1,\tau_2}, X^{\alpha_2,\tau_2}]_\mp \right\rangle} = \left(G^1_{\alpha_1\alpha_2} \right)^{-1} \equiv g^{\alpha_1}(\tau_1 - \tau_2)^{-1} \tag{3.32}$$

(Note: in case of different sites, there would be an additional δ_{ij} for the site index. For two Hubbard operators, the (anti-)commutator is time independent).
The equation has to be understood in the sense that $\left(G^1_{\alpha_1\alpha_2} \right)^{-1} G^1_{\alpha_1\alpha_2} = \delta_{\tau_1 - \tau_2}$.
The last definition is done to get accordance to Slobodyans paper.
One can generalize this equation of motion. Initially one notes, that the λ_α came only from the derivative of the Hubbard operator. If one constrains the derivative to the Θ functions, i.e. $\partial_\tau \to \partial_\tau^\Theta$ one can derive the more general formula

$$\left(g_0^{\alpha_i \alpha_j} \right)^{-1} G_0^{(n)} = \left[-\partial_{\tau_i}^\Theta G_0^{(n)} \right]_j, \tag{3.33}$$

where the $[]_j$ means a reduction to time arguments of the form $\tau_i - \tau_j$. Now one uses the RHS of equation (3.33) on equation (3.29). First one looks at the only two terms, in which two specific times τ_i (the one from the time derivative) and τ_j are directly next to each other. This has to be, because the Θ functions only

connect directly neighboring operators. The two term naturally differ in their order, so one has

$$\left[-\partial_{\tau_i}^{\Theta} G_0^n\right]_j = \delta(\tau_i - \tau_j)\left([\ldots]\left\langle \ldots X^{\alpha_i}(\tau_i)X^{\alpha_j}(\tau_j)\ldots\right\rangle \pm [\ldots]\left\langle \ldots X^{\alpha_j}(\tau_j)X^{\alpha_i}(\tau_i)\ldots\right\rangle\right)$$
(3.34)
$$= \delta(\tau_i - \tau_j)[\ldots]\left\langle \ldots [X^{\alpha_i}, X^{\alpha_j}]_{\mp}(\tau_j)\ldots\right\rangle.$$
(3.35)

The $[\ldots]$ are products of Θ functions that only contain times $\tau_k \neq \tau_i$. Now this can be done with all other operators by summing over j and replacing the derivative by equation (3.33)

$$\left(g_0^{\alpha_i}\right)^{-1} G_0^{(n)} = \sum_j -\delta(\tau_i - \tau_j)[\ldots]\left\langle \ldots [X^{\alpha_i}, X^{\alpha_j}]_{\mp}(\tau_j)\ldots\right\rangle \qquad (3.36)$$

If one brings the $g_0^{\alpha_i \alpha_j}$ over to the other side, one can integrate over τ_i from $-\beta$ to τ_i. One knows the solution for the special case, namely that all times are equal. In this case the product of Hubbard operators can be evaluated directly. The result is in accordance to the generalized Wick's theorem:

$$G_0^n(\alpha_1 \ldots \alpha_{2n}) = \sum_j (\pm)^{j+i} g_0^{\alpha_i \alpha_j}(\tau_i - \tau_j) \times$$
(3.37)
$$\times \left\langle X^{\alpha_1}(\tau_1), \ldots, X^{\alpha_{j-1}}(\tau_{j-1})[X^{\alpha_j}, X^{\alpha_i}]_{\pm}(\tau_j)X^{\alpha_{j+1}}(\tau_{j+1})\ldots X^{\alpha_n}(\tau_n)\right\rangle.$$
(3.38)

In the above equation, the Hubbard operator with index i is separated out and what is left are time ordered products of $n-1$ operators. This can be brought into the form in Slobodyans paper by remembering the sign convention for the Green's function.

Attention!!! With Wick's theorem, diagonal Hubbard operators of the form $\left(X^{00} - X^{11}\right)(\tau)$ are created. From the basic equations of motion is is clear, that these are time-independent, i.e.

$$X^{nn}(\tau) = X^{nn}(0). \qquad (3.39)$$

These operators are nonetheless tagged with a time and are subject to time-ordering. Thus they cannot be neglected in the further reduction of the problem!

One mainly uses Wick's theorem to break down product of averages of Hubbard operators into sums of products of simpler functions and weighting factors. It is still quite cumbersome to apply Wick's theorem for bigger products. For bosons additional signs are created by the commutators, whereas for fermions the ordering creates new signs just by itself. So for the case of bosons one can use a graphical method that helps with the book-keeping of all the appearing factors.

3.2 Direct Checks on simple examples

3.2.1 Free Bosons

One has to check, whether the generalized Wick's theorem works for simple cases. Especially it has to converge to the well-known, regular Wick's theorem for $U \to 0$. To this end we calculate first the one-particle Green's function:

$$\left\langle T_\tau \hat{b}^\dagger(\tau_1) \hat{b}(\tau_2) \right\rangle = \left\langle T_\tau \sum_{n=0}^\infty \sum_{n'=0}^\infty \sqrt{n+1} \sqrt{n'+1} X^{n+1,n} X^{n',n'+1} \right\rangle. \quad (3.40)$$

One knows that in Fourier representation after analytical continuation

$$\left\langle X^{n+1,n} X^{n',n'+1} \right\rangle = \delta_{n,n'} \frac{\langle X^{n,n} \rangle - \langle X^{n+1,n+1} \rangle}{\beta(\omega - \epsilon)}. \quad (3.41)$$

For the free case, $\langle X^{n,n} \rangle$ is given by

$$\langle X^{n,n} \rangle = \frac{e^{-n\beta\epsilon}}{Z}, \qquad Z = \sum_{n=0}^\infty e^{-n\beta\epsilon} = \frac{1}{1 - e^{-\beta\epsilon}}. \quad (3.42)$$

So (3.40) reduces to

$$\left\langle T_\tau \hat{b}^\dagger(\tau_1) \hat{b}(\tau_2) \right\rangle = \frac{1}{Z} \sum_{n=0}^\infty (n+1) \frac{e^{-n\beta\epsilon} - e^{-(n+1)\beta\epsilon}}{\beta(\omega - \epsilon)}. \quad (3.43)$$

One just have to evaluate the sums with the sum rule for geometric series

$$\sum_{n=0}^\infty e^{-n\beta\epsilon} = \frac{1}{1 - e^{-\beta\epsilon}} = Z \qquad \sum_{n=0}^\infty n e^{-n\beta\epsilon} = \frac{\partial \sum_{n=0}^\infty e^{-n\beta\epsilon}}{\partial(-\beta\epsilon)} = \frac{\partial}{\partial(-\beta\epsilon)} Z \quad (3.44)$$

$$\sum_{n=0}^\infty (n+1) e^{-(n+1)\beta\epsilon} = \sum_{n=0}^\infty n e^{-n\beta\epsilon} = \frac{\partial}{\partial(-\beta\epsilon)} Z \quad (3.45)$$

Putting all together we get that

$$\left\langle T_\tau \hat{b}^\dagger(\tau_1) \hat{b}(\tau_2) \right\rangle = \frac{1}{Z} \frac{Z + \frac{\partial}{\partial(-\beta\epsilon)} Z - \frac{\partial}{\partial(-\beta\epsilon)} Z}{\beta(\omega - \epsilon)} = \frac{1}{\beta(\omega - \epsilon)}. \quad (3.46)$$

One can apply a similar calculation to a product containing more than two operators. One can focus the discussion on the part that connects two specific times, τ and τ'

$$\left\langle \ldots \hat{b}^\dagger \tau \ldots \hat{b} \tau' \ldots \right\rangle = \left\langle \cdots \sum_n \sqrt{(n+1)} X^{n+1,n}(\tau) \cdots \sum_{n'} \sqrt{(n'+1)} X^{n',n'+1}(\tau') \ldots \right\rangle. \quad (3.47)$$

At this point one uses Wick's theorem. For the sake of clarity the other contractions of $\hat{b}^\dagger(\tau)$ with other times are ommited. One then has

$$\left\langle \cdots \sum_n \sqrt{(n+1)} X^{n+1,n}(\tau) \cdots \sum_{n'} \sqrt{(n'+1)} X^{n',n'+1}(\tau') \ldots \right\rangle =$$
(3.48)

$$\sum_n g^{n+1,n}(\tau - \tau') \left\langle \cdots \sum_n \sqrt{(n+1)} \sum_{n'} \sqrt{(n'+1)} \delta_{n,n'} \left(X^{n,n} - X^{n+1,n+1} \right)(\tau') \right\rangle$$
(3.49)

Now one uses, that in the limit $U \to 0$, $g^{n+1,n}(\tau - \tau') = g^{1,0}(\tau - \tau') = G^0(\tau - \tau')$. The sum over n' can be dropped and because both components of the commutator are evaluated at the same time, the overall sum reduces to

$$\sum_{n=0}^{\infty} (n+1) \left(X^{n,n} - X^{n+1,n+1} \right) = \sum_{n=0}^{\infty} X^{n,n} = I(\tau').$$
(3.50)

Since the identity is time-independent and invariant under time ordering it can be dropped and one has

$$\left\langle \ldots \hat{b}^\dagger \tau \ldots \hat{b} \tau' \ldots \right\rangle = G^0(\tau - \tau') \left\langle \ldots \right\rangle_{/\tau/\tau'} + \text{Contractions with other terms.}$$
(3.51)

This is how the regular Wick's theorem is supposed to work for noninteracting particles. What happens if we try to reduce two creation operators with each other, e.g.

$$\left\langle \ldots \hat{b}^\dagger \tau \ldots \hat{b}^\dagger \tau' \ldots \right\rangle?$$
(3.52)

In this case, one has first the contribution

$$\left\langle \cdots \sum_n \sqrt{(n+1)} X^{n+1,n}(\tau) \cdots \sum_{n'} \sqrt{(n'+1)} X^{n'+1,n'}(\tau') \ldots \right\rangle$$
(3.53)

$$= \sum_{n,n'=0}^{\infty} \sqrt{(n+1)(n'+1)} g_0^{n+1,n}(\tau - \tau') \left\langle \ldots \left(\delta_{n',n+1} X^{n+2,n} - \delta_{n,n'+1} X^{n+1,n-1} \right)(\tau') \ldots \right\rangle$$
(3.54)

Again, in the free case, $g_0^{n+1,n} = g_0^{1,0}$ for all n and one can focus on the Hubbard term only.

$$= \sum_{n,n'=0}^{\infty} \sqrt{(n+1)(n'+1)} \delta_{n',n+1} X^{n+2,n} - \delta_{n,n'+1} X^{n+1,n-1}$$
(3.55)

$$= \sum_{n=0}^{\infty} \sqrt{(n+1)(n+2)} X^{n+2,n} - \sum_{n=1}^{\infty} \sqrt{(n+1)n} X^{n+1,n-1}$$
(3.56)

If one replaces the sum over n in the second term over the new variable $n' = n-1$, the second sum becomes the first, but just with a minus. This means, that all $g_0^{10}(\tau - \tau')$ and hence all g_0^{20} contributions drop out of the final equation. There

must be an exact cancelation for the g_0^{20} terms. This is what one would expect for the free particles given the well-known Wick's theorem. This is an important benchmark for any serious theory expanding the use of creation and annihilation operators.

3.2.2 Direct check for a product of three Hubbard operators

The best check is still to apply the generalized Wick's theorem for a simple situation that can be followed easily. The smalles possible combination that is non-trivial consists of three Hubbard operators and looks as follows

$$\left\langle T_\tau X^{01}(\tau_1) X^{12}(\tau_2) X^{20}(\tau_3) \right\rangle = \mathrm{e}^{\lambda_{20}\tau_3 - \lambda_{21}\tau_2 - \lambda_{10}\tau_1} \left(\Theta(123) b^0 + \Theta(231) b^1 + \Theta(312) b^2 \right) \tag{3.57}$$

The b^n are the probabilities of a site being occupied by n particles according to a Boltzmann distribution $b^n = \mathrm{e}^{-\beta\epsilon(n)}/Z$. The three probabilities satisfy the relation

$$b^0 = \mathrm{e}^{\beta\lambda_{10}} b^1 = \mathrm{e}^{\beta\lambda_{10}} \mathrm{e}^{\beta\lambda_{21}} b^2 = \mathrm{e}^{\beta\lambda_{20}} b^2 \qquad \text{since } \lambda_{20} = \lambda_{21} + \lambda_{10}. \tag{3.58}$$

Straightforward application of Wick's theorem leads to

$$\left\langle T_\tau X^{01}(\tau_1) X^{12}(\tau_2) X^{20}(\tau_3) \right\rangle = \tag{3.59}$$

$$g^{20}(\tau_3 - \tau_2) g^{10}(\tau_2 - \tau_1) \left(b^0 - b^1 \right) - g^{20}(\tau_3 - \tau_1) g^{21}(\tau_1 - \tau_2) \left(b^1 - b^2 \right). \tag{3.60}$$

One can rewrite the free locators as

$$g^{ij}(\tau) = \frac{\mathrm{e}^{\lambda_{ij}\tau}}{(\mathrm{e}^{\beta\lambda_{ij}} - 1)} \left(\Theta(\tau) + \Theta(-\tau) \mathrm{e}^{\beta\lambda_{ij}} \right) \tag{3.61}$$

One first has to check, whether the time exponential is $\mathrm{e}^{\lambda_{20}\tau_3 - \lambda_{21}\tau_2 - \lambda_{10}\tau_1}$ in all terms. In the first term one has to use that $\lambda_{10}\tau_2 - \lambda_{20}\tau_2 = -\lambda_{21}\tau_2$. A similar relation holds true for τ_1 in the second term. The remainder is then

$$\frac{1}{\mathrm{e}^{\beta\lambda_{20}} - 1} \left(\Theta(31) + \Theta(13) \mathrm{e}^{\beta\lambda_{20}} \right) \left(\frac{\left(b^0 - b^1 \right)}{\mathrm{e}^{\beta\lambda_{10}} - 1} \left(\Theta(21) + \Theta(12) \mathrm{e}^{\beta\lambda_{10}} \right) + \frac{\left(b^1 - b^2 \right)}{\mathrm{e}^{\beta\lambda_{21}} - 1} \left(\Theta(12) + \Theta(21) \mathrm{e}^{\beta\lambda_{21}} \right) \right) \tag{3.62}$$

For $\tau_1 > \tau_2 > \tau_3$ this becomes with $b^1 = \mathrm{e}^{-\beta\lambda_{10}} b^0$ and $b^2 = \mathrm{e}^{-\beta\lambda_{20}} b^0$

$$\frac{\mathrm{e}^{\beta\lambda_{20}}}{\mathrm{e}^{\beta\lambda_{20}} - 1} \left(\frac{1 - \mathrm{e}^{-\beta\lambda_{10}}}{\mathrm{e}^{\beta\lambda_{10}} - 1} \mathrm{e}^{\beta\lambda_{10}} - \frac{\mathrm{e}^{-\beta\lambda_{10}} - \mathrm{e}^{-\beta\lambda_{20}}}{\mathrm{e}^{\beta\lambda_{21}} - 1} \right) b^0 \tag{3.63}$$

Using that $\frac{1 - \mathrm{e}^{-\beta\lambda_{10}}}{\mathrm{e}^{\beta\lambda_{10}} - 1} \mathrm{e}^{\beta\lambda_{10}} = 1$ and that $-\frac{\mathrm{e}^{-\beta\lambda_{10}} - \mathrm{e}^{-\beta\lambda_{20}}}{\mathrm{e}^{\beta\lambda_{21}} - 1} = -\mathrm{e}^{-\beta\lambda_{20}} \frac{\left(\mathrm{e}^{\beta\lambda_{21}} - 1 \right)}{\left(\mathrm{e}^{\beta\lambda_{21}} - 1 \right)} = -\mathrm{e}^{-\beta\lambda_{20}}$ one finds that indeed for this time constellation the time exponential is multiplied with b_0. The same holds true for the other time combination. (During the project Wick's theorem for 4 Hubbard operators was calculated, but the results are too lengthy to include here).

3.3 Wick's theorem applied to physical systems

This part gives a scheme that shows, how Hubbard operators can be applied to physical systems and how the cumulant expansion (see appendix) can be applied to find the last remaining terms. This is taken mostly from Sloboyans paper [74]. Let us assume, that the Hamiltonian can be decomposed into

$$H \equiv= H_0 + H_{int} = \sum_i h_i + \sum_{i<j} v_{ij}. \tag{3.64}$$

The Hamiltonian is then separated into individual groups(sites) indexed by i, which are eigenfunctions of the unperturbed Hamiltonian

$$h_i \left| i, p \right\rangle = \lambda_p \left| i, p \right\rangle. \tag{3.65}$$

The Hubbard operators are then constructed as

$$X_i^{pq} = \left| i, p \right\rangle \left\langle i, q \right|, \tag{3.66}$$

with the properties

$$X_i^{pq} X_i^{rs} = \delta_{qr} X_i^{ps} \tag{3.67}$$

$$(X_i^{pq})^\dagger = X_i^{qp}, \sum_p X_i^{pp} = 1 \tag{3.68}$$

$$\left[X_i^{pq}, X_j^{rs} \right]_\mp = \delta_{ij} \{ \delta_{qr} X_i^{ps} \mp \delta_{ps} X_i^{rq} \}. \tag{3.69}$$

One uses the commutator if both or one of the operators is of Bose type, otherwise one uses the anticommutator. One can establish the type of operator by observing the expression of the Hubbard operator in creation and annihilation operators. If they can be expressed by an odd number of Fermion creation operators, they are of Fermi type.(Because the way a creation operator can be decomposed into Hubbard operators is not dependent on the interaction strength, this property is conserved under a change of interaction strength.)

The Hamiltonian can then be rewritten with Hubbard operators

$$H = \sum_{ip} \lambda_{ip} X_i^{pq} + \sum_{i<j} \sum_{pqrs} B_{ij}^{pqrs} X_i^{pq} X_j^{rs}, \tag{3.70}$$

where

$$B_{ij}^{pqrs} = \left\langle pi, rj | \nu | qi, sj \right\rangle. \tag{3.71}$$

Further it was assumed that $\lambda_{ip} = \lambda_p$. For the correlation functions one needs the statistical means of the Hubbard operators in Heisenberg representation

$$\tilde{X}(\tau) = e^{H\tau} X e^{-H\tau}, \qquad (0 < \tau < \beta = 1/kT) \tag{3.72}$$

$$X(\tau) = e^{H_0\tau} X e^{-H_0\tau}, \qquad (0 < \tau < \beta = 1/kT). \tag{3.73}$$

In the interaction representation, these terms can be reexpressed as

$$\left\langle T \tilde{X}_1^{\alpha_1}(\tau_1) \dots \tilde{X}_n^{\alpha_n} \right\rangle = \left\langle T X_1^{\alpha_1}(\tau_1) \dots X_n^{\alpha_n} \sigma(\beta) \right\rangle_0 / \left\langle \sigma(\beta) \right\rangle_0, \tag{3.74}$$

where

$$\langle\ldots\rangle_0 = \mathrm{Tr}\ (\rho_0\ldots)\,, \rho = \mathrm{e}^{-\beta H_0}/\mathrm{Tr}\ \mathrm{e}^{-\beta H_0}, \tag{3.75}$$

whereas $\langle\ldots\rangle$ is the average with respect to the full Hamiltonian. The temperature scattering matrix is given by

$$\sigma(\beta) = \mathrm{e}_T^{-\int_0^\beta H_{int}(\tau)\,d\tau} = \sum_{n=0}^\infty \frac{(-1)^n}{n!}\int_0^\beta d\tau_1\ldots\int_0^\beta d\tau_n T\{H_{int}(\tau_1)\ldots H_{int}(\tau_n)\}. \tag{3.76}$$

One easily sees that

$$X_i^{pq}(\tau) = \mathrm{e}^{\lambda_{pq}\tau}X_i^{pq}, \qquad \lambda_{pq} = \lambda_p - \lambda_q. \tag{3.77}$$

At this point, the generalized version of Wick's theorem can be used. The expansion of the mean value of the T product of Hubbard operators with respect to commutators and anticommutators of the non-diagonal operator $\alpha = pq, p \neq q$ can be done stopped when one of two cases happens. One ends with a one point Green's function

$$\langle T_\tau X^{10}(\tau_1)X^{01}(\tau_2)\rangle = \Theta(12)\langle X^{11}\rangle + \Theta\langle X^{00}\rangle \tag{3.78}$$

or

$$\langle T_\tau X^{01}(\tau_1)X^{10}(\tau_2)\rangle = \Theta(12)\langle X^{00}\rangle + \Theta\langle X^{11}\rangle \tag{3.79}$$

or a time-independent product of commutators of diagonal Hubbard operators

$$\left\langle \prod_j \left(X^{j_1 j_1} - X^{j_2 j_2}\right) \right\rangle. \tag{3.80}$$

These products can be very simply evaluated:
Since the groups(sites) are independent in the original Hamiltonian, it is sufficient to look at the averages of operators from one group(site) only

$$\left\langle (X^{\alpha_1})^{N_1}\ldots(X^{\alpha_k})^{N_k}\right\rangle_0 = \left(\frac{\partial^{N_1}}{\partial\eta_1^{N_1}}\frac{\partial^{N_2}}{\partial\eta_k^{N_2}}\cdots\frac{\partial^{N_k}}{\partial\eta_k^{N_k}}\left\langle \exp\left(\sum_i \eta_i X^{\alpha_i}\right)\right\rangle_0\right)\Bigg|_{\{\eta_i=0\}} \tag{3.81}$$

where $\alpha = p_i p_i$. The off-diagonal parts are already taken out with Wick's theorem. The remaining averages can be evaluated using the equation (3.67). It immediately shows that averages vanish, unless all α_i are the same. Because of the projector property, the final terms are always $\pm\langle X^\alpha\rangle$. This is a special case of the more general cumulant expansion, which is described in more detail in the appendix.

3.4 Graphical evaluation of the Products

The goal is to find a way to keep track of all appearing terms in the evaluation of averages of the form

$$\left\langle T\{\prod X_k^{pq}\}\right\rangle_0. \tag{3.82}$$

One has to evoke the generalized Wick's theorem to reduce the order of the product. It is given by (3.19). For now one needs only to consider averages of

products X^α, with $\alpha = i, i+1$ or $i+1, i$, i.e. simple creations and annihilations of a single particle.

There exist some rules for simplifying the calculations with bosons

1. In each product, the number of creations and annihilations must be equal. Otherwise the conservation of particles would not be fulfilled.

2. The contraction happens only within Hubbard operators of the same lattice site. This follows immediately from the Wick's theorem, as $g_{0i}^\alpha \sim \delta_{0i}$. It should be clear, the different sites behave independently.

3. Reshuffle all operators such that operators with the same site index are next to each other.

From the equation

$$\left\langle X^{12}(\tau_1) X^{21}(\tau_2) \right\rangle = \left\langle X^{22} - X^{11} \right\rangle g^{12}(\tau_1 - \tau_2) = \left\langle X^{11} - X^{22} \right\rangle g^{21}(\tau_2 - \tau_1)$$
$$(3.83)$$

one gets the symmetry relation $g^{pq}(\tau) = -g^{qp}(-\tau)$. A closer inspection shows, that for a given product, only time arguments of equal operators can be permutated with each other, otherwise inconsistencies occur.

One can use a mnemonic device similar to the usual diagrammatic techniques to keep track of the resulting terms within one group. The technique uses charged arrows. One starts with horizontal lines representing the occupation numbers of the site and arrows representing the corresponding Hubbard operators according to the time they appear. For example, for the case of $\left\langle X^{12}(\tau_1) X^{21}(\tau_2) X^{23}(\tau_3) X^{32}(\tau_4) \right\rangle_0$ one can draw (see figure 1):

Figure 3.1:

1. Each arrow carries a charge. The charge of an up-arrow is +1, the one of a down-arrow is -1.

2. Each arrowhead can only move on its own line. The tip of an arrow can only connect to an end of another arrow. The same holds true for the bottom of an arrow.

3. Each time an arrow is created, it obtains the time of the added arrow. The charge of an arrow can be seen from the distance of its two endpoints.

4. To avoid multiple countings, it is convenient to stick to enlarging one arrow until the charge hits zero.

5. One should enlarge one arrow by using all possible ways of connecting another arrow piece. This can be done either by moving the head, or by moving the buttom. This creates an additional $-$ sign.

6. Every time an arrowhead connects to an arrow bottom, the formula is multiplied with the propagator $g_i^{pq}(\tau_1 - \tau_2)$ of the moving arrow (taken from the endpoints). The time argument is the difference between the connecting (τ_1) and the connected time (τ_2). A similar thing holds for the bottom of an arrow, but the propagator obtains an extra minus. (Since one start with a positively charged arrow and end every time one hits zero there is a stop, there is no need for further rules regarding the motion of downward arrows.)

7. If an arrow connects to another arrow, and the resulting charge is zero, a bucket is created (see figure 3.2). The bucket has still a time argument, denoted by the time of the connected arrow (the handle is pointing at the right time). Upon creation of a bucket, only a regular propagator is produced. Afterwards one continues with another up-arrow.
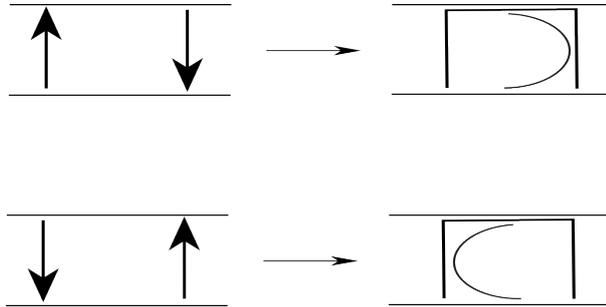
Figure 3.2:

8. A bucket cannot be moved, however another arrow can connect to it. This can happen in three different ways. However for all three cases, the bucket is used up, denoted by completing the circle within, as seen in figure 3.3 . The three cases are:

   - **a)** The up arrow is on the same level as the bucket. This results an an additional -2 to the propagator, the arrow is conserved and moves to the bucket.
   - **b)** The arrow is on the level below the bucket. Here, no additional sign is gathered. But the arrow still moves to obtain the time of the bucket.
   - **c)** The arrow is on the level above the bucket. The usual propagator gains a -1. The arrow moves to the bucket and gets a new time.
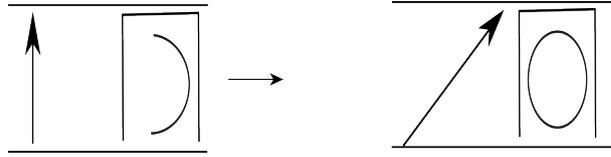
Figure 3.3:

9. Starting from one arrow, one has to connect it in all the ways possible. One stops when there are only buckets left. Then one starts over with the remaining combinations.

10. At the end average over the **product** of all the remaining **open** buckets. Each gives a factor $\left(X^{ii} - X^{jj}\right)$, where the i is the lower level of the bucket and the j is the upper level.

Example: One can use the rules to find the expression for $\left\langle X^{12}(\tau_1)X^{21}(\tau_2)X^{23}(\tau_3)X^{32}(\tau_4)\right\rangle_0$. The starting point can be seen in figure 3.1. Starting with the first up-arrow at time τ_2, one has two possibilities of connecting the head further. In the first case it moves to the left and recombining to zero with the down arrow to the left. One therefore gains a factor $g^{21}(\tau_2 - \tau_1)$ and a bucket with time τ_1.

Figure 3.4:

Since zero was just hit, one has to start over with the remaining up-arrow. It has two choices. For once it can create another bucket with the down arrow at time τ_3. This produces a factor $g^{32}(\tau_4 - \tau_3)$. Now only buckets are left (see figure 3.5), so one can average over them, since they are all open. This gives the factor $\left\langle \left(X^{00} - X^{11}\right)\left(X^{11} - X^{22}\right)\right\rangle$

So the total contribution is
$g^{21}(\tau_2 - \tau_1)g^{32}(\tau_4 - \tau_3)\left\langle \left(X^{11} - X^{22}\right)\left(X^{22} - X^{33}\right)\right\rangle_0$.
Next comes the second way of connecting the second up-arrow. It can close the first bucket. It gains the time τ_1 itself and the overall contribution gets an additional $-g^{32}(\tau_4 - \tau_1)$ multiplied, because the connecting arrow is one level above the bucket. The result can be seen in figure 3.6.
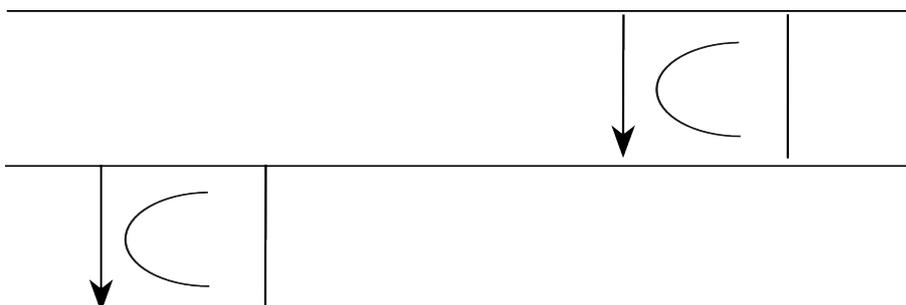
Figure 3.5:
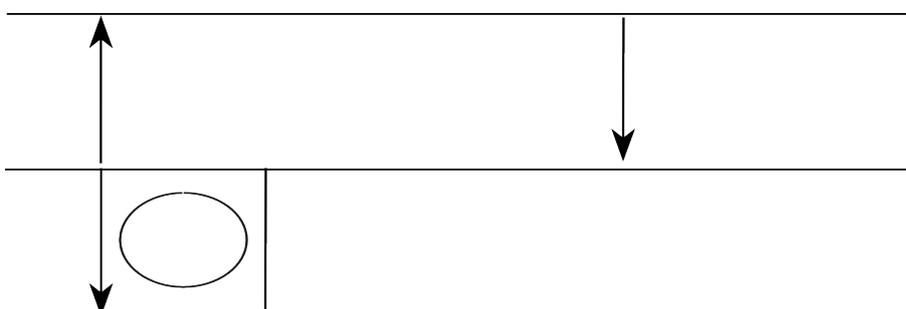
Figure 3.6:

The only option left is creating an open bucket in the top level. Because this destroys the last up-arrow, one has to average to get the total contribution
$$-g^{21}(\tau_2 - \tau_1)g^{32}(\tau_4 - \tau_1)g^{32}(\tau_1 - \tau_3)\left\langle X^{11} - X^{22}\right\rangle.$$

Now we have to start over again. Instead of combining the τ_2 up-arrow with an down-arrow, one enlarges it using the up-arrow at τ_4. This gives the propagator $g^{21}(\tau_2 - \tau_4)$. This way a +2-charged arrow is created (figure 3.7)
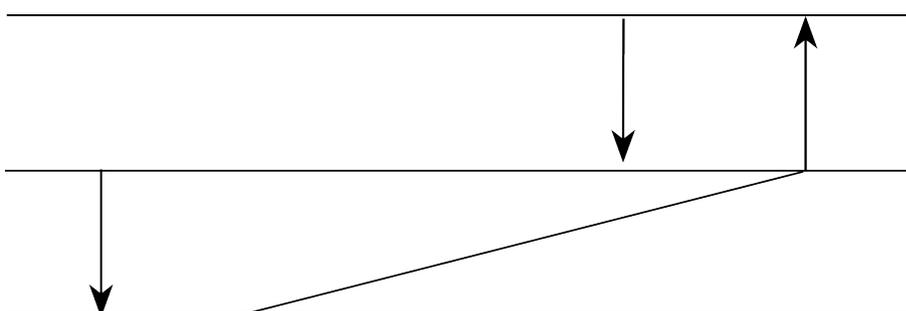
Figure 3.7:

Again one is at a crossroad. The first choice is to move the tip to create a +1-charged arrow at time τ_3. Since it is a +2 charged arrow, the propagator changes to $g^{31}(\tau_4 - \tau_3)..$
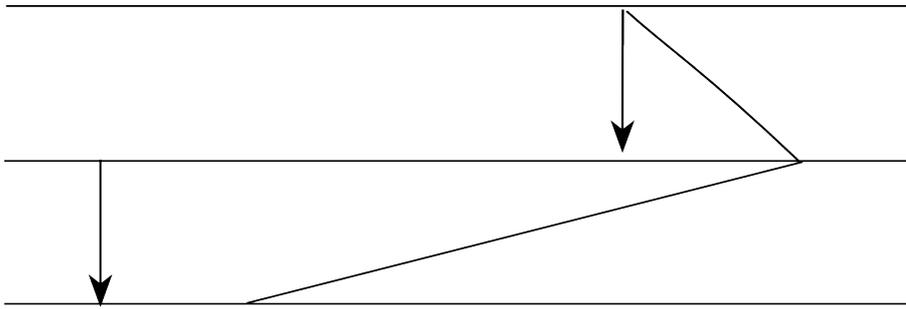
Figure 3.8:

The last recombination $g^{21}(\tau_3 - \tau_1)$ creates another open bucket. The remainder has to be averaged and the total contribution is $g^{21}(\tau_2 - \tau_4)g^{31}(\tau_4 - \tau_3)g^{21}(\tau_3 - \tau_1)\langle(X^{11} - X^{22})\rangle$.

The last contribution one gets by alternatively moving the bottom of the large arrow instead of the tip, thereby creating a factor $-g^{31}(\tau_4 - \tau_1)$.
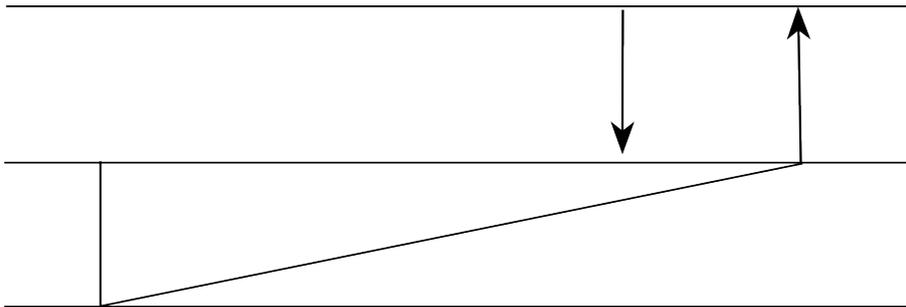
Figure 3.9:

Now one can again only move the tip of this $+1$ arrow $(g^{32}(\tau_1 - \tau_3))$. An open bucket is created and by definition one gets the remaining contribution $(X^{22} - X^{33})$.
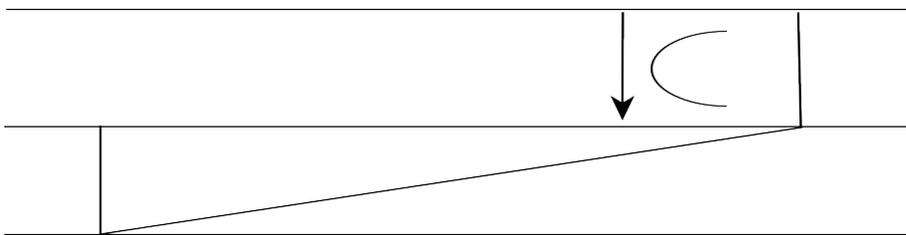
Figure 3.10:

So the last contribution is $-g^{21}(\tau_2-\tau_4)g^{31}(\tau_4-\tau_1)g^{21}(\tau_1-\tau_3)\left\langle X^{22}-X^{33}\right\rangle_0$. To sum up all the contributions, one gets

$$\left\langle X^{12}(\tau_1)X^{21}(\tau_2)X^{23}(\tau_3)X^{32}(\tau_4)\right\rangle_0 = \tag{3.84}$$

$$g^{21}(\tau_2-\tau_1)g^{32}(\tau_4-\tau_3)\left\langle\left(X^{11}-X^{22}\right)X^{22}-X^{33}\right\rangle_0 \tag{3.85}$$

$$-g^{21}(\tau_2-\tau_1)g^{32}(\tau_4-\tau_1)g^{32}(\tau_1-\tau_3)\left\langle X^{11}-X^{22}\right\rangle \tag{3.86}$$

$$g^{21}(\tau_2-\tau_4)g^{31}(\tau_4-\tau_3)g^{21}(\tau_3-\tau_1)\left\langle X^{11}-X^{22}\right\rangle \tag{3.87}$$

$$-g^{21}(\tau_2-\tau_4)g^{31}(\tau_4-\tau_1)g^{21}(\tau_1-\tau_3)\left\langle X^{22}-X^{33}\right\rangle_0 \tag{3.88}$$

With these rules, one can find the contribution of each product of averages of bosonic operators.

3.5 Connectedness

It is important for future applications of Hubbard operators to assert, whether a connectedness theorem is valid or not. This means that to the exact propagator, only connected diagrams contribute, i.e.

$$G_{\alpha\beta} \equiv \frac{-1}{\langle\sigma\rangle}\left\langle T_\tau\left[X^\alpha(\tau)X^\beta(\tau')\sigma\right]\right\rangle = -\left\langle T_\tau\left[X^\alpha(\tau)X^\beta(\tau')\sigma\right]\right\rangle_{con} \tag{3.89}$$

with $\sigma = T_\tau\exp\{-\int_0^\beta V(\tau)\,d\tau\}$.

The numerator in equation (3.89) is a sum of terms. It is necessary for the connectedness theorem, that the terms containing more than one annihilation (i.e. the diagramm contains more than one loop) factorize. For the case of non-interacting particles this is trivially fulfilled by the Wick's theorem, which doesn't apply in it's original form here.
One has to differenciate between the different contributions of each diagram. First there are diagrams with closed buckets (where an creation Hubbard operator contracted with a commutator) and those without. The ones without closed buckets have direct equivalents, whereas the closed bucket terms do not. These terms can then be grouped again into the ones where the time arguments propagate from one external time to the other, or where they take a shorter path and the remainder forms a bubble.
At this point one makes the **hypothesis**, that for low temperatures, the closed bucket diagrams vanish. It will be shown for a two-legged diagram, but so far a proof for general n-leg diagrams is not there yet.
If this hypothesis was true, it would still not be sufficient to show, that only connected diagrams survive. In the following it is shown, that for low temperatures the connectedness theorem still holds, provided that out assumption about the open bucket diagrams is true.
So for the non-closed bucket diagrams, the propagators do indeed factor, however one is stuck with terms of the sort

$$\left\langle\prod_i\left[X^{\alpha_i},X^{\beta_i}\right]_\mp\right\rangle = \left\langle\prod_i\left(X^{i,i}\mp X^{i+1,i+1}\right)\right\rangle. \tag{3.90}$$

So for the theorem to work, these terms should factor as well. However, here is a problem. Taken for instance

$$\left\langle \left(X^{i,i} + X^{i+1,i+1} \right)^2 \right\rangle =^? \left\langle X^{i,i} + X^{i+1,i+1} \right\rangle^2. \qquad (3.91)$$

The right hand side conveniently reduces to $(b^i)^2 + 2b^i b^{i+1} + (b^{i+1})^2$. Here $b^i = \frac{e^{-\beta\lambda_i}}{\sum_k e^{-\beta\lambda_k}}$.

The left hand side can be rewritten as $\left\langle (X^{i,i})^2 \right\rangle + \left\langle X^{i,i} X^{i+1,i+1} \right\rangle + \left\langle X^{i+1,i+1} X^{i,i} \right\rangle + \left\langle X^{i+1,i+1} X^{i+1,i+1} \right\rangle$.

Since $(X^{i,i})^2 = X^{i,i}$ one could guess that $\left\langle (X^{ii})^2 \right\rangle = \left\langle X^{ii} \right\rangle$. From the cumulant expansion one knows that

$$\left\langle X^{ii} X^{ii} \right\rangle = \left\langle X^{ii} X^{ii} \right\rangle_{con} + \left\langle X^{ii} \right\rangle_{con} \left\langle X^{ii} \right\rangle_{con} = \frac{\partial}{\partial(-\beta\lambda_i)} b^i + b^i = b^i - (b^i)^2 + (b^i)^2 = b^i, \qquad (3.92)$$

so our assumption is indeed true. Also $\left\langle X^{ii} X^{i+1,i+1} \right\rangle_{con} = -b^i b^{i+1}$. For equation (3) this gives then

$$b^i + b^{i+1} =^? (b^i)^2 + 2b^i b^{i+1} + (b^{i+1})^2, \qquad (3.93)$$

which in general is not true. This however forbids, that the terms cancel as nicely as in the usual applications. Especially in the expansion (as can be seen later for the calculations on the models), prefactors of the form β^n appear from the disconnected diagrams. These powers of β diverge for $T \to 0$, so one has to show, that the remainder converges to 0 even faster.

One can see, that in the second order expansion (see below), the disconnected factor is weighted by (It should be remembered, that in this notation b^i_j, the i is the state and j the site index) $\left((b^0_1 - b^1_1)^2 (b^0_2 - b^1_2)^2 - \left(b^0_1 + b^1_1 \right) \left(b^0_2 + b^1_2 \right) \right)$. This term vanishes as $T \to 0$, since b^1 and b^0 approach 1 or 0. If one can show that

$$\lim_{\beta\to\infty} \left(\left\langle \prod_i \left(X^{i,i} - X^{i+1,i+1} \right) \right\rangle - \prod_i \left\langle X^{i,i} - X^{i+1,i+1} \right\rangle \right) = 0, \qquad (3.94)$$

then the connectedness theorem holds in the zero temperature limit. Morover, if this term approaches zero fast enough, all low temperature divergencies of the form β^n will be unproblematic.

One can reduce the problem by noting that the averages on different sites vanish. One can also tentatively ignore terms standing for higher occupations than 1. This is not necessary and it is later obvious why these terms vanish. One is left with the problem for operators of the kind $\left\langle (X^0 - X^1)^n \right\rangle$. The right hand side of (3.94) simply becomes then $(-\text{sgn}(\epsilon))^n$.

For the left hand side one can calculate (cross-terms vanish for the Hubbard operators)

$$\left\langle \left(X^0 - X^1 \right)^n \right\rangle = \sum_{k=0}^n \binom{n}{l} \left\langle (X^0)^1 (-X^1)^{(n-k)} \right\rangle = \left\langle X^0 \right\rangle + (-1)^n \left\langle X^1 \right\rangle \quad (3.95)$$

For the last equality one used that $(X^{nn})^l = X^{nn}$.

Now

$$\left(b^0 - b^1\right)^n - \left((b^0)^n + (-b^1)^n\right) = \sum_{k=1}^{n-1} \binom{n}{l} (b^0)^l (-b^1)^{n-l} \le \binom{n}{n/2} (n-2) \, b^0 b^1.$$
(3.96)

The last product vanishes exponentially for $T \to 0$. So one doesn't need to worry about divergencies in the low temperature regime. Since Wick's theorem otherwise applies just like the one for the usual creation and annihilation operator, it is obvious that in the low temperature regime, all disconnected controbution vanish. This is, because otherwise all diegramms have the same combinatorial factors as in the well known case.

One can also see that higher occupations like X^2 also lead to products im the cumulant expansion that factor into b_2, which also vanish exponentially (even faster due to the repulsion). Hence our assumption of neglecting higher occupations is well justified.

This section shows, that the generalized locator expansion technique is particularily effective in the forward scattering approximation. Here, disconnected diagrams do not show up, so the results are good for arbitrary U and T, as long as the locator expansion itself is valid. One can in this case introduce the generalized locator

$$L_i(\mathrm{i}\omega) = \sum_{n=0}^{\infty} \frac{n+1}{\mathrm{i}\omega - (\epsilon_i - 2Un)} \left(b_i^n - b_i^{n+1}\right).$$
(3.97)

In the forward scattering approximation, any Green's function can be written as a product of the locators of all the sites of the contributing path and the tunneling constants, which do not have to be the same for all sites (especially in the case of magnetic fields).

Chapter 4

Applications of the Technique

In the following we want to apply the generalized locator expansion to several simple systems.

4.1 Application to Lowest Order Tunneling/ Forward Scattering

For some physical quantities it is already enough to know the correlation function of a chain of sites. Here no loops and the such are considered. We are especially interested in the difference between hard-core bosons and fermions. The matrix elements for the lowest order tunneling between $n+1$ sites are given by

$$\left\langle T_\tau \{ X_{n+1}^{i,i+1} X_1^{j+1,j} \prod_{k=1}^{n} \left(X_{k+1}^{r_{k+1}+1,r_{k+1}} X_k^{r_k,r_k+1} \right) \} \right\rangle_0 \tag{4.1}$$

The k could be different atoms or different states on the same site (that are not interacting with each other). The sum can obviously be devided into n independent couples of lattice site operators. Since one has only single site bubbles, one does not need to worry about additional $-$ signs for fermions. Hence the overall contribution is

$$\prod_{k=1}^{n} g_k^{i_k+1,i} \times \left\langle \prod_{k=1}^{n} \left(X_k^{i_k,i_k} \mp -X_k^{i_k+1,i_k+1} \right) \right\rangle_0 , \tag{4.2}$$

given the connecting indices are the same, i.e. meaning that a particle jumps exactly into the state from which is later jumps out again. Otherwise no rings could be formed by the arrows. Since the product in (4.2) is over independent Hubbard operators it decomposes into

$$\left\langle \prod_{k=1}^{n} \left(X_k^{i_k,i_k} - X_k^{i_k+1,i_k+1} \right) \right\rangle_0 = \prod_{k=1}^{n} \left(\left\langle X_k^{i_k,i_k} \right\rangle_0 \mp \left\langle X_k^{i_k+1,i_k+1} \right\rangle_0 \right) \tag{4.3}$$

In the case of hard-core particles, only the zeroth and first occupation need to be taken into account. Hence the main contribution takes the form

$$\prod_{k=1}^{n} g_k^{i_k+1,i} \prod_{k=1}^{n} \left(\left\langle X_k^{0,0} \right\rangle_0 - \left\langle X_k^{1,1} \right\rangle_0 \right) \tag{4.4}$$

For the bosonic case and $T \to 0$, one has that $\prod_{k=1}^{n} \left(\left\langle X_k^{1,1} \right\rangle_0 - \left\langle X_k^{0,0} \right\rangle_0 \right) = \prod_{k=1}^{n} \mathrm{sgn}(\epsilon_k)$. Now it is convenient to go to the frequency representation (see equation (3.26)) by performing the Fourier transform and the analytic continuation. The result is

$$G^R(\omega) = -\mathrm{i} \prod_{k=1}^{n} -\frac{J_{k+1,k} \mathrm{sgn}(\epsilon_k)}{\epsilon_k - \omega}. \tag{4.5}$$

Fermions on the other hand behave according to

$$G^R(\omega) = -\mathrm{i} \prod_{k=1}^{n} \frac{J_{k+1,k}}{\epsilon_k - \omega}. \tag{4.6}$$

This result was predicted by Müller [75] on heuristic grounds and could be proven with this technique systematically. It shows, that there is indeed a difference between hard-core bosons and fermions, even though they have the same occupation statistics.

4.2   Hopping between two sites

The following parts are restricted to bosons. An important form of hopping is the back and forth hopping between two sites $(1 \to 2 \to 1)$. It is crucial for estimating contributions of diagrams that vary in space by an additional 1-loop. In this section all diagrams are calculated and it is shown that the closed-bucket terms go to zero as $T \to 0$.

This contribution is given by the following expression

$$J^2 \int_0^\beta \int_0^\beta \left\langle X_1^{01}(\tau') X_1^{10}(\tau_2) X_2^{01}(\tau_2) X_1^{01}(\tau_1) X_2^{10}(\tau_1) X_1^{10}(\tau) \right\rangle d\tau_1 d\tau_2, \tag{4.7}$$

where J is the hopping constant. The goal is to find this term in frequency representation. The Fourier transformations are defined selfconsistently and dimensionless

$$g(\tau) = \sum_n g^{10}(\omega_n) \mathrm{e}^{\mathrm{i}\omega_n \tau} \qquad g^{10}(\omega_n) = \frac{1}{\beta} \int_0^\beta g(\tau) \mathrm{e}^{-\mathrm{i}\omega_n \tau}. \tag{4.8}$$

For the matrix element one uses, that the averaged product factors into the different sites

$$\left\langle X_1^{01}(\tau') X_1^{10}(\tau_2) X_2^{01}(\tau_2) X_1^{01}(\tau_1) X_2^{10}(\tau_1) X_1^{10}(\tau) \right\rangle = \left\langle X_1^{01}(\tau') X_1^{10}(\tau_2) X_1^{01}(\tau_1) X_1^{10}(\tau) \right\rangle \left\langle X_2^{01}(\tau_2) X_2^{10}(\tau_1) \right\rangle \tag{4.9}$$

The second term decomposes with the generalized Wick's theorem to

$$g_2^{10}(\tau_1 - \tau_2) \left(b_2^0 - b_2^1 \right). \tag{4.10}$$

The first term becomes

$$g_1^{10}(\tau - \tau') g_1^{10}(\tau_2 - \tau_1)(b_1^0 + b_1^1) \tag{4.11}$$

$$+g_1^{10}(\tau_2 - \tau') g_1^{10}(\tau - \tau_1)(b_1^0 + b_1^1) \tag{4.12}$$

$$-2g^{10}(\tau_2 - \tau') g^{10}(\tau - \tau') g^{10}(\tau' - \tau_1) \left(b_1^0 - b_1^1 \right) \tag{4.13}$$

$$-2g^{10}(\tau_2 - \tau_1) g^{10}(\tau - \tau_1) g^{10}(\tau_1 - \tau') \left(b_1^0 - b_1^1 \right) \tag{4.14}$$

All of these terms multiplied by $g_2^{10}(\tau_1 - \tau_2)\left(b_2^0 - b_2^1\right)$ can be represented by Feynmanlike diagrams (see figure (4.1)).
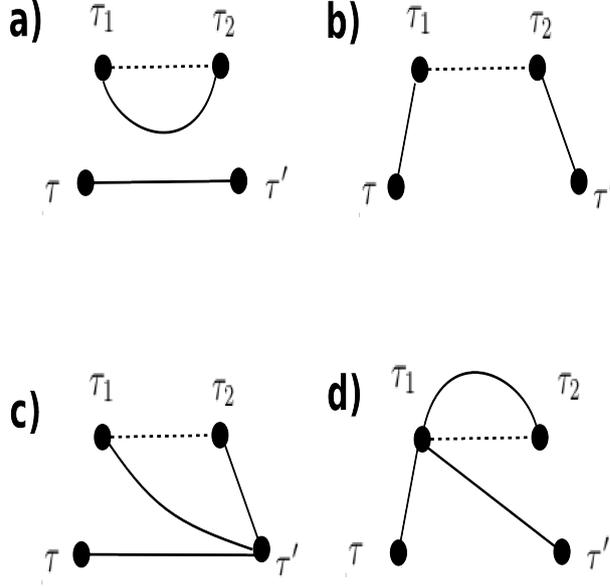
Figure 4.1: The relevant diagrams for one hop: a) disconnected diagram b) connected diagram c) and d) closed-bucket diagrams. The dashed lines are locators on site 2, the drawn out lines for site 1

The first term is the disconnected term.

$$J^2 \int_0^\beta \int_0^\beta d\tau_1 d\tau_2 g_1^{10}(\tau - \tau')g_1^{10}(\tau_2 - \tau_1)g_2^{10}(\tau_1 - \tau_2)(b_1^0 + b_1^1)\left(b_2^0 - b_2^1\right) \quad (4.15)$$

One can evoke the theory of Matsubara sums to deal with the disconnected part.

$$\int_0^\beta \int_0^\beta g_1^{10}(\tau_2 - \tau_1)g_2^{10}(\tau_1 - \tau_2)d\tau_2 d\tau_1 = \beta^2 \sum_n g_1^{10}(\omega_n)g_2^{10}(\omega_n) \quad (4.16)$$

$$= -\beta\left(\frac{n(\lambda_2)}{\lambda_2 - \lambda_1} + \frac{n(\lambda_1)}{\lambda_1 - \lambda_2}\right) \quad (4.17)$$

$n(\epsilon)$ in this equation denotes the Bose function $1/\left(e^{\beta\epsilon} - 1\right)$. The Fourier transform with respect to $\tau - \tau'$ of the function $g_1^{10}(\tau - \tau') = -\left[\beta\left(i\omega - \lambda\right)\right]^{-1}$ and the Fourier transform of the first term is

$$\frac{J^2}{\omega + i0 - \lambda_1}\left(\frac{n(\lambda_2)}{\lambda_2 - \lambda_1} + \frac{n(\lambda_1)}{\lambda_1 - \lambda_2}\right)(b_1^0 + b_1^1)\left(b_2^0 - b_2^1\right) \quad (4.18)$$

The second term is the connected diagram and a convolution. So the product just decomposes into the product of the Fourier transforms

$$\frac{J^2}{\beta} \left(\frac{1}{\omega + i0 - \lambda_1} \right)^2 \frac{1}{\omega + i0 - \lambda_2} \left(b_1^0 + b_1^1 \right) \left(b_2^0 - b_2^1 \right) \tag{4.19}$$

For the third term one substitutes the Fourier transform $g(\tau) = \sum_n g(\mathrm{i}\omega_n) \mathrm{e}^{\mathrm{i}\omega_n \tau}$ and gets

$$J^2 \sum_{n,n_1,n_2,n_3} \int_0^\beta \int_0^\beta d\tau_1 d\tau_2 g_1^{10}(\mathrm{i}\omega_{n_1}) g_1^{10}(\mathrm{i}\omega_n) g_1^{10}(\mathrm{i}\omega_{n_2}) g_2^{10}(\mathrm{i}\omega_{n_3}) \times \tag{4.20}$$

$$\times \mathrm{e}^{\mathrm{i}\omega_{n_1}\left(\tau_2-\tau'\right)+\mathrm{i}\omega_n(\tau-\tau')+\mathrm{i}\omega_{n_2}(\tau'-\tau_1)+\mathrm{i}\omega_{n_3}(\tau_1-\tau_2)}. \tag{4.21}$$

One can see, that the integration over τ_1 gives the factor $\beta\delta_{n_3,n_2}$ and the τ_2 integration gives $\beta\delta_{n_1,n_3}$. The remainder is

$$J^2 \beta^2 \sum_{n,n_1} \left(g_1^{10}(\mathrm{i}\omega_{n_1}) \right)^2 g_1^{10}(\mathrm{i}\omega_n) g_2^{10}(\mathrm{i}\omega_{n_1}) \mathrm{e}^{\mathrm{i}\omega_n\left(\tau-\tau'\right)} \tag{4.22}$$

This in return means, that the Fourier transform of the third term with respect to $(\tau - \tau')$ can be directly read off

$$-2J^2 \beta^2 g_1^{10}(\mathrm{i}\omega_n) \sum_{n_1} \left(g_1^{10}(\mathrm{i}\omega_{n_1}) \right)^2 g_2^{10}(\mathrm{i}\omega_{n_1}) \left(b_1^0 - b_1^1 \right) \left(b_2^0 - b_2^1 \right). \tag{4.23}$$

One can calculate the sum easily with computer programs such as *Mathematica* to see that

$$\sum_n \left(g_1^{10}(\mathrm{i}\omega_n) \right)^2 g_2^{10}(\mathrm{i}\omega_n) = \frac{\left(\sinh(\beta\lambda_1/2)^{-2} \left(\lambda_1 - \lambda_2 + \sinh(\beta\lambda_1)/\beta \right) - \sinh(\beta\lambda_2/2)^{-2} \right)}{4\beta \left(\lambda_1 - \lambda_2 \right)} \tag{4.24}$$

The fourth term can be also calculated by including the Fourier transforms

$$J^2 \sum_{n_1,n_2,n_3,n_4} \int_0^\beta \int_0^\beta d\tau_1 d\tau_2 g_1^{10}(\mathrm{i}\omega_{n_1}) g_1^{10}(\mathrm{i}\omega_{n_2}) g_1^{10}(\mathrm{i}\omega_{n_3}) g_2^{10}(\mathrm{i}\omega_{n_4}) \times \tag{4.25}$$

$$\times \mathrm{e}^{\mathrm{i}\omega_{n_1}(\tau_2-\tau_1)+\mathrm{i}\omega_{n_2}(\tau-\tau_1)+\mathrm{i}\omega_{n_3}(\tau_1-\tau')+\mathrm{i}\omega_{n_4}(\tau_1-\tau_2)} \tag{4.26}$$

The integration gives the factor $\beta^2 \delta(n_3+n_4, n_1+n_2)\delta(n_1, n_4) = \beta^2 \delta(n_3, n_2)\delta(n_1, n_4)$. This reduces the term to

$$J^2 \beta^2 \sum_{n_1,n_2} g_1^{10}(\mathrm{i}\omega_{n_1}) g_2^{10}(\mathrm{i}\omega_{n_1}) \left(g_1^{10}(\mathrm{i}\omega_{n_2}) \right)^2 \mathrm{e}^{\mathrm{i}\omega_{n_2}\left(\tau-\tau'\right)} \tag{4.27}$$

From this, one can directly read off the Fourier transformation

$$-2J^2 \beta^2 \left(g_1^{10}(\mathrm{i}\omega_{n_2}) \right)^2 \left(\sum_{n_1} g_1^{10}(\mathrm{i}\omega_{n_1}) g_2^{10}(\mathrm{i}\omega_{n_1}) \right) \left(b_1^0 - b_1^1 \right) \left(b_2^0 - b_2^1 \right) \tag{4.28}$$

Also, the sum can be evaluated using specialized computational programs to give

$$\left(\sum_{n_1} g_1^{10}(\mathrm{i}\omega_{n_1}) g_2^{10}(\mathrm{i}\omega_{n_1})\right) = \frac{(\coth(\beta\lambda_2/2) - \coth(\beta\lambda_1/2))}{2\beta\left(\lambda_1 - \lambda_2\right)} \qquad (4.29)$$

Taking the limit process $\beta \to \infty$ shows, that both closed-bucket diagrams vanish in the limit of small temperatures! This makes the application of the technique particularily easy. The connected diagrams can be easily evaluated using standard Feynman rules, whereas the disconnected diagrams are cancelled by the denominator for low temperatures, as shown in the previous chapter.

4.3 Interference between two paths at low temperatures

To investigate the effect of multiple path interference, one takes a simple model of 4-sites, where the connection between the initial site i and the final site f happen over two possible intermediate sites, 1 and 2. The coupling Hamiltonian is given by

$$H_{int} = -J\left(X_1^{10}X_i^{01} + X_2^{10}X_i^{01} + X_f^{10}X_1^{01} + X_f^{10}X_2^{01}\right) + c.c. \qquad (4.30)$$

To lowerst order, in the Green's function appear terms of order J^2. The involved terms are explicitly written in the Hamiltonian. Pictorally, the particle can use the upper path or the lower path. From the expansion one knows that the largest contribution is given by

$$G_{fi}^1(\tau - \tau') = \frac{1}{2}\int_0^\beta\int_0^\beta \left\langle X_f^{01}X_i^{10}H_{int}(\tau_1)H_{int}(\tau_2)\right\rangle d\tau_1\, d\tau_2. \qquad (4.31)$$

From the rules for the evaluation of products, it is clear, that only four terms contribute, because all other terms either do not conserve the particle number. For instance, for path one one has

$$\left\langle X_f^{01}(\tau')X_i^{10}(\tau)X_1^{10}(\tau_1)X_i^{01}(\tau_1)X_f^{10}(\tau_2)X_1^{01}(\tau_2)\right\rangle + \qquad (4.32)$$

$$\left\langle X_f^{01}(\tau')X_i^{10}(\tau)X_f^{10}(\tau_1)X_1^{01}(\tau_1)X_1^{10}(\tau_2)X_i^{01}(\tau_2)\right\rangle \qquad (4.33)$$

Since these terms factor the same according to the rules, the integration gives the same result for both. The same is obviously true for the second path. After taking the Fourier transform and the standard calculation one gets the result

$$G_{fi}^1(\omega) = \frac{J^2}{\beta}\left(\frac{(b_i^0 - b_i^1)(b_1^0 - b_1^1)(b_f^0 - b_f^0)}{(\omega - \epsilon_i)(\omega - \epsilon_1)(\omega - \epsilon_f)} + \frac{(b_i^0 - b_i^1)(b_2^0 - b_2^1)(b_f^0 - b_f^1)}{(\omega - \epsilon_i)(\omega - \epsilon_2)(\omega - \epsilon_f)}\right). \qquad (4.34)$$

Both terms contribute equally, but the contribution depends on the occupation of the paths. This was expected. Because $(b^0 - b^1)/(\omega - \epsilon) = -\mathrm{sgn}(\epsilon)(\omega - \epsilon)$, one can see that for low temperatures and low frequencies, the two paths always interfere constructively! This is what one would expect for bosons.

4.4   Corrections to the Single Particle Green's function

In equation (4.5) the forward scattering approximation for the single particle Green's function for bosons was calculated. What kind of corrections com to mind? The simplest correction is a "side-step" to site j in real space that deviates from the forward scattering approximation between sites i and f like in figure (4.2).
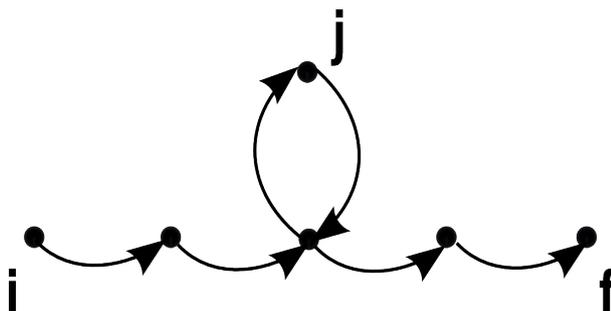
Figure 4.2:

From the previous calculations in the section about the hopping between two sites it is already clear, that for very low temperatures one only has to consider the connected diagrams. This means the diagram with the side-step to site j is in frequency representation and for the lowest excitation is reduced by the factor

$$J^2 \frac{1}{(\omega - \epsilon_j)(\omega - \epsilon_{j-1})} \frac{\left(b_{j-1}^0 + b_{j-1}^1\right)}{\left(b_{j-1}^0 - b_{j-1}^1\right)} \left(b_j^0 - b_j^1\right) = J^2 \frac{\text{sgn}(\epsilon_j)}{\omega - \epsilon_j} \frac{\text{sgn}(\epsilon_{j-1})}{\omega - \epsilon_{j-1}}. \quad (4.35)$$

$j - 1$ is of course the site the jump is starting from. One can see, that for bosons typically, these side-steps enhance the function. Because J is very small compared to ϵ, these corrections are suppressed. However the number of these contributions grows linearly with the length of the chain that is considered. If one denotes the number of nearest neighbors that are not in the original chain themselves with d, then the number of possible side steps is proportional to Ld. Then the amplitude of the sum of all corrections compared to the forward scattering approximation is given by

$$C_{RS} = \frac{LdJ^2}{W^2}, \quad (4.36)$$

where W is the bandwidth of the distribution of the on-site energies. This means, there exists a length-scale, where these contributions dominate over the forward scattering approximation. It is given by

$$L_{RS} = \frac{W^2}{dJ^2}. \quad (4.37)$$

The index RS denotes here real space contributions.

With the new help of the Hubbard operators one can find another correction to the forward scattering approximation, that also scales linearly with L. But instead of side-stepping in real space, the deviation is in Fock-space. One can find a heuristic explanasion of this. If a site along the chain is occupied, there are two possible ways to continue. Either the particle moves away from the site, which is the case in the forward scattering approximation. However, there is also the low chance, that one particle hops on top of the other. Of course, this contribution is strongly suppressed, but the number of events like this scales linearily with the length of the chain (or to be more precise with the number of occupied sites). Each of these side-steps in Fock space give a contribution that has a factor

$$2\frac{\langle X^{21}X^{12}\rangle}{\langle X^{10}X^{01}\rangle}(\omega) = 2\frac{\omega - \epsilon}{\omega - (\epsilon + U)}\frac{(b^1 - b^2)}{(b^0 - b^1)}. \tag{4.38}$$

The factor 2 stems from the prefactor of the Hubbard operator in the decomposition of the creation and annihilation operators. Since $U >> \epsilon$ and for a contributing path $\epsilon < 0$, one has that $b^1 = 1, b^0 \approx b^2 \approx 0$. This means that the contribution pro path is roughly $2W/U$. This means, that these contributions enhance the spreading. One could in principle look for higher contributions, but the prefactor $b^i - b^{i+1}$ is only for $i = 0, 1$ non-negligible. If the chemical potential is shifted with respect to the middle of the bandwidth W by an amount η (in units of W), then the fraction of occupied states along a chain is $(1/2 - \eta)$. This means, that the Fock-space deviations scale like

$$C_{FS} = 2\frac{W(1/2 - \eta)L}{U}. \tag{4.39}$$

This means the length scale over which these dominate over the forward scattering approximation is then given by

$$L_{FS} = \frac{U}{W(1 - 2\eta)}. \tag{4.40}$$

η is positive when the chemical potential is shifted towards the lowe end of the band. For $\eta = 1/2$, the band is completely empty and the probability for occupied states is zero, so Fock-space contributions become negligible.
The competition between real space and Fock space deviations is given by the factor

$$\frac{C_{RS}}{C_{FS}} = \frac{UdJ^2}{W^3(1 - 2\eta)}. \tag{4.41}$$

If one denotes the Green's function in the forward scattering approximation as G_0, then for larger L the corrected Green's function is given by

$$G(L) = \left(1 + \frac{LdJ^2}{W^2} + \frac{W(1 - 2\eta)L}{U}\right)G_0 \tag{4.42}$$

Chapter 5

Experimental Relevance

There still remains the question of how, if possible, one can observe these strong interaction effects. First of all it is easier to control interactions in a real space setting. In the introduction experiments that worked with dynamical localization were described, but here the interactions are rather difficult to change. However, recently Anderson localization in real space were observed by Kondov et. al. [76]. They used laser light that was scattered by a diffuser to superimpose a quasi random optical field on top of the trap, where they could observe the Anderson localization afterwards. In this setup, the intensity of the superimposed laser light can be used to control the band width W. Since the effect of the spatial deviations as well as the effects of the Fock space deviations depend on the band width, but in a different way, there could open up a possibility to observe these features.

What about the interactions? In cold gases, only very few scattering processes are allowed (in bosonic gases this is s-wave scattering). Because all of those interactions are elastic, they can in fact be described by one parameter, namely the phase change during a scattering event. This means, that at low temperatures, every interaction between two particles can be described by a pseudo potential

$$U(\vec{r}) = \frac{2\pi\hbar^2 a}{m}\delta(\vec{r}).$$

(5.1)

Here m is the mass of the scattering particles and the new quantity a is the so called scattering length that completely describes elastic scattering. To influence the scattering length one Feshbach resonances as described in [77] and [78]. During scattering, normally only one scattering channel is used at low temperatures. The energy profile looks typically like a Born-Oppenheimer molecular potential as seen in the lower graph in figure (5.1)

However, energetically above the open channel are typically other channels that are closed, because they involve scattering of different hyperfine states. One typical potential curve for a closed channel is the upper graph in figure (5.1). Due to the particular shape of the interaction potential, the well of the closed channel can be of the same energy as the incoming particles. If they come closer
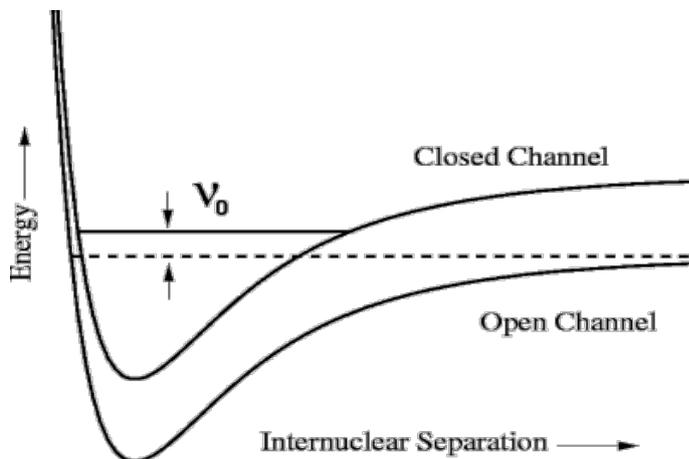
Figure 5.1: Two particle interaction potential at Feshbach resonance, image taken from [79]

in energy, these two channels couple to each other. Particular resonances are achieved, when the energy of the incoming particles is in accordance with the energy of a bound state of the forbidden channel. At this point, the scattering length diverges. As mentioned before, the forbidden channels typically consists of different hyperfine transitions than the open channel. Hyperfine states are often susceptible to Zeeman shifts when a magnetic field is applied. This means, that when the open and the closed channel have different signs in the Zeeman shift, one can shift the energy of the channels relative to each other by applying magnetic fields. This way one can tune the energy of the bound states of the closed channel via the magnetic field to be on resonance with the energy of the incoming particles at a critical magnetic field B_c. This is a Feshbach resonance. Because the behaviour close to resonance is universal, one can describe it by simple equations. Quite generally the scattering length close to transition behaves as

$$a = a_{bg}\left(1 - \frac{\Delta_B}{B - B_c}\right),\tag{5.2}$$

where a_{bg} is the background scattering length of the open channel and Δ_B the width of the Feshbach resonance, which is determined by channel-specific properties. At the Feshbach transition, the sign of the scattering length changes. On one side one has attractive potentials (here molecules can form), whereas the other side is repulsive, as seen in figure (5.2). Which side is which depends on the hyperfine structure of the resonance.

With this tool at hand one can control the interactions of atomic gases carefully. One can see, that close to the transition,

$$\frac{1}{U} \sim \frac{m\left(B - B_c\right)}{2\pi\hbar^2\Delta_B}\tag{5.3}$$

An this way the Green's function with Fock space deviations can be written as
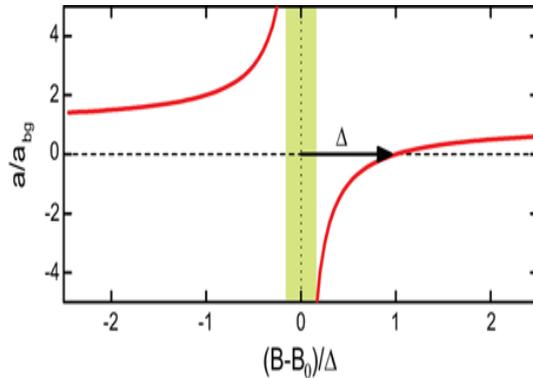
Figure 5.2: Behaviour of scattering length at Feshbach resonance, image taken from [80]

$$G(B,L) = \left(1 + \frac{LdJ^2}{W^2} + \frac{W(1-2\eta)Lm\,(B-B_c)}{2\pi\hbar^2\Delta_B}\right)G_0. \qquad (5.4)$$

One typically defines the localization length as

$$\xi^{-1}(\omega) = \lim_{L\to\infty} \frac{1}{L}\left\langle \ln\left(\frac{G^R(L,\omega)}{G(1,\omega)}\right)\right\rangle. \qquad (5.5)$$

To observe localization one usually lets a small cloud of atoms spread out over the disordered potential. Since one is interested in many body physics it is maybe suitable to first let a cloud of atoms spread homogeneously in an "empty" trap at a certain magnetic field and afterwards superimpose the random potential. This way one creates a disordered bath of particles with constant chemical potential (at least within the trap dimensions). Now one would have to move a second cloud of cold atomic matter to the center of the trap and let it spread out. It would be this cloud that would localize in the disordered, but occupied potential. After some time one could measure the integrated column density via atomic absorption processes to obtain a density field of the matter from which the background matter field can be subtracted. The remaining peak should fall of exponentially at larger distances from the center of the trap. Given that a decrease interaction opens higher channels in Fock space for expansion, the cloud size will most likely be bigger for lower U or larger $(B-B_c)$ The localization length measured this way is $\xi(0)$. According to equation (5.5) and the fact that the corrections of the Green's function grow only linearly in L, one would expect that far away from the center the localization length is independent of the magnetic field (at least if one stays on the repulsive side of the Feshbach resonance).

This experimental challenges for this setup are very hard, but within the reach of current technology. However it remains very questionable, whether meaningful measurements could be performed, because the measurements for ξ would have to be evaluated far away from the trap center, where the fluctuations of the background create a strong noise term. However these are not principle

limitations, which gives hope that other experimental setups could make use of the generalized locator expansion.

Chapter 6

Conclusion and Outlook

In this thesis a new powerful technique for dealing with interactive bosonic insulators and some fermionic systems has been introduced. It is centered around the fact, that the usual creation and annihilation operators can be expanded in terms of Hubbard operators.

Hubbard operators have the advantage of being diagonal in the interaction Hamiltonian, which makes their time evolution easily trackable. The downside is that they do not obey the usual (anti)-commutation relations and thus are not subject to Wick's theorem either.

One part of the project was to find an alternative to Wick's theorem that applies to Hubbard operators (and beyond). This generalized Wick's theorem had to be proven and tested. It was verified, that the classical Wick's theorem can be recovered in the limit of a vanishing interaction $U \to 0$.

It became pretty clear that more diagrams are then created with the usual Wick's theorem. To make handling the contractions easier, a new mnemonic device, the arrow scheme, was developed. It can be immediately seen, which diagrams have classical counterparts and which one arise because of the Hubbard operators alone.

The next important step was to show that the diagrams that have classical analogons obey a connectedness theorem in the limit of low temperatures. This means that, provided the non-classical diagrams are vanishing as well, the disconnected diagrams cancel and only the connected diagrams are needed for the evaluation of correlation functions. One can even define generalized locators that make the evaluation of forward scattering amplitudes very easy.

For the particular case of 4-legged diagrams it was demonstrated, that the new diagrams do vanish for small temperatures. However a direct check for 6-legged diagrams or a proof for n-leg diagrams remains open. So far it is only known that all the new diagrams contain multifold poles, so that a theory that describes all of them seems possible.

The new technique was then applied to the simple case of forward scattering, thereby supporting the predictions by Müller through a direct calculation. It shows, that there are indeed differences between hard-core bosons and fermions on the level of Green's functions. This is in fact a remarkable result given that the occupation statistics are almost identical.

In the step, correction to the forward scattering approximation were calculated. These corrections are due to deviations in real space from the shortest path

and due to deviations in Fock-space from the shortest path (see figure (6.1)). Both of these contributions enhance the overall Green's function. This is rather surprising because the corrections in Fock-space are proportional to U^{-1} and to the number of occupied sites. This means that lowered repulsion leads to a better spreading! However the explanation is fairly intuitive. The lower the interaction, the more paths for particle transport open up. That this concept makes sense can be seen on the example of repulsively bound atom pairs, which do not move in free space [81]. In that case, a lack of channels to seperate the highly energized atom pairs prevents them from splitting.
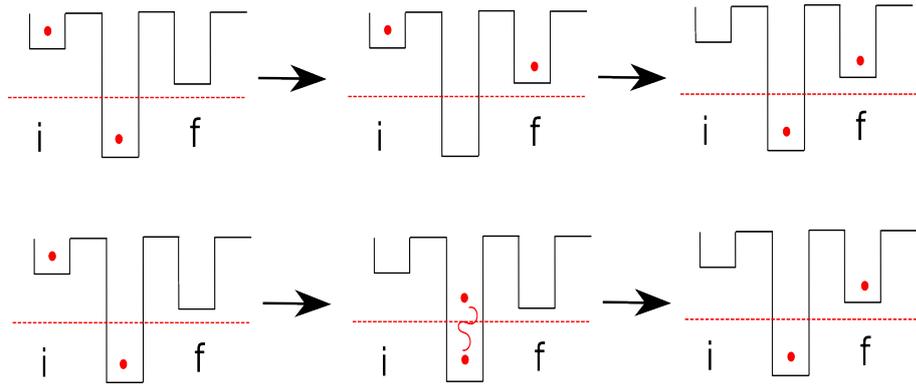
Figure 6.1: Hopping of a boson from site i to f. The red dashed line represents the chemical potential μ. The upper panel shows the only allowed path for hard-core bosons. The lower path shows a deviation in Fock space where the intermediate site is doubly occupied. This path is penalized by $1/U$ and completely forbidden for true hard-core bosons.

Nevertheless, a direct quantitative observation based on single particle Green's function seems prohibitive.
But these limits can be overcome with this technique as well. It is a matter of straightforward calculation of the 6-legged diagrams of Hubbard operators to allow for the evaluation of the density-density correlation function. The density-density correlation function can then be used to make more quantitative predictions, that are likely to yield results that can be used in correlation experiments with cold matter.
Another strength of this technique is that it can be expanded straightforwardly. This is done by defining more complex Hubbard operators, that not only describe the interaction within single states (that can be occupied by multiple particles) but also within groups of states that have interactions between them. This can be used to model for instance the interactions between fermions or sites with a complex inner structure, that contain many possible interacting states. As such one also has to solve the issue of whether a certain Hubbard operator is bosonic or fermionic nonambiguously. This technique should also provide a convenient starting point for numerical calculations of more complex systems.

Chapter 7

Appendix

.1 Useful commutators for bosons

$$\left[\hat{a},(\hat{a}^\dagger)^n\right] = n(\hat{a}^\dagger)^{n-1} \qquad \left[\hat{a}^\dagger,(\hat{a})^n\right] = -n\hat{a}^{n-1} \tag{1}$$

$$\left[\hat{a},\mathrm{e}^{\alpha\hat{a}^\dagger}\right] = \alpha\mathrm{e}^{\alpha\hat{a}^\dagger}, \qquad \mathrm{e}^{-\alpha\hat{a}^\dagger}\hat{a}\mathrm{e}^{\alpha\hat{a}^\dagger} = \hat{a}+\alpha \tag{2}$$

$$\mathrm{e}^{-\alpha\hat{a}^\dagger}\mathrm{e}^{\beta\hat{a}}\mathrm{e}^{\alpha\hat{a}^\dagger} = \mathrm{e}^{\beta\alpha}\mathrm{e}^{\beta\hat{a}} \qquad \mathrm{e}^{\alpha\hat{a}^\dagger\hat{a}}\hat{a}\mathrm{e}^{-\alpha\hat{a}^\dagger\hat{a}} = \mathrm{e}^{-\alpha}\hat{a} \tag{3}$$

$$\left[\hat{a}^j,(\hat{a}^\dagger)^j\right] = \sum_{l=0}^{j-1}\hat{a}^l\left[\hat{a},(\hat{a}^\dagger)^j\right]\hat{a}^{j-1-l} \tag{4}$$

This is shown by induction using the relation $[AB,C] = A\,[B,C] + [A,B]\,C$.

Let $\left[\hat{a},\left[\hat{a},(\hat{a}^\dagger)^j\right]\right]_0 = \left[\hat{a},(\hat{a}^\dagger)^j\right]$ and $\left[\hat{a},\left[\hat{a},(\hat{a}^\dagger)^j\right]\right]_n = \left[\hat{a},\left[\hat{a},(\hat{a}^\dagger)^j\right]_{n-1}\right]$.

Theorem:

$$\left[\hat{a},\left[\hat{a},(\hat{a}^\dagger)^j\right]\right]_n = \frac{j!}{(j-1-n)!}(\hat{a}^\dagger)^{j-1-n} \text{ for } n < j \tag{5}$$

Proof by induction: Induction start:

$$\left[\hat{a},\left[\hat{a},(\hat{a}^\dagger)^j\right]\right]_0 = j(\hat{a}^\dagger)^{j-1} = \frac{j!}{(j-1-0)!}(\hat{a}^\dagger)^{j-1-0} \tag{6}$$

Induction step:

$$\left[\hat{a},\left[\hat{a},(\hat{a}^\dagger)^j\right]\right]_{n+1} = \left[\hat{a},\left[\hat{a},(\hat{a}^\dagger)^j\right]_n\right] = \left[\hat{a},\frac{j!}{(j-1-n)!}(\hat{a}^\dagger)^{j-1-n}\right] \tag{7}$$

$$= \frac{j!}{(j-1-n)!}\left[\hat{a},(\hat{a}^\dagger)^{j-1-n}\right] = \frac{j!\,(j-1-n)}{(j-1-n)!}(\hat{a}^\dagger)^{j-1-n-1} \tag{8}$$

$$= \frac{j!}{(j-1-(n+1))!}(\hat{a}^\dagger)^{j-1-(n+1)} \tag{9}$$

Theorem:

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$$\hat{a}^l \left[\hat{a}, (\hat{a}^\dagger)^j \right] = \sum_{k=0}^{l} \binom{l}{k} \left[\hat{a}, \left[\hat{a}, (\hat{a}^\dagger)^j \right] \right]_k \hat{a}^{l-k} \tag{10}$$

Proof by induction; induction start $\hat{a} \left[\hat{a}, (\hat{a}^\dagger)^j \right] = \hat{a} \left[\hat{a}, \left[\hat{a}, (\hat{a}^\dagger)^j \right] \right]_0 = \left[\hat{a}, \left[\hat{a}, (\hat{a}^\dagger)^j \right] \right]_1 +$
$\left[\hat{a}, \left[\hat{a}, (\hat{a}^\dagger)^j \right] \right]_0 \hat{a} = \sum_{k=0}^{1} \left[\hat{a}, \left[\hat{a}, (\hat{a}^\dagger)^j \right] \right]_0 \hat{a}^{1-k}$
Induction step

$$\hat{a}^{l+1} \left[\hat{a}, (\hat{a}^\dagger)^j \right] = \hat{a} \left(\sum_{k=0}^{l} \binom{l}{k} \left[\hat{a}, \left[\hat{a}, (\hat{a}^\dagger)^j \right] \right]_k \hat{a}^{l-k} \right) \tag{11}$$

$$= \sum_{k=0}^{l} \binom{l}{k} \left(\left[\hat{a}, \left[\hat{a}, (\hat{a}^\dagger)^j \right] \right]_{k+1} + \left[\hat{a}, \left[\hat{a}, (\hat{a}^\dagger)^j \right] \right]_k \hat{a} \right) \hat{a}^{l-k} \tag{12}$$

$$= \sum_{k=0}^{l+1} \binom{l+1}{k} \left[\hat{a}, \left[\hat{a}, (\hat{a}^\dagger)^j \right] \right]_k \hat{a}^{l+a-k} \tag{13}$$

It was used, that $\binom{n}{k} = \binom{n-1}{k-1} + \binom{n-1}{k}$
Plugging these identities together one arrives at

$$\left[\hat{a}^j, (\hat{a}^\dagger)^j \right] = \sum_{l=0}^{j-1} \hat{a}^l \left[\hat{a}, (\hat{a}^\dagger)^j \right] \hat{a}^{j-1-l} = \sum_{l=0}^{j-1} \sum_{k=0}^{l} \binom{l}{k} \left[\hat{a}, \left[\hat{a}, (\hat{a}^\dagger)^j \right] \right]_k \hat{a}^{j-1-k} \tag{14}$$

$$= \sum_{l=0}^{j-1} \sum_{k=0}^{l} \binom{l}{k} \frac{j!}{(j-1-k)!} (\hat{a}^\dagger)^{j-1-k} \hat{a}^{j-1-k} \tag{15}$$

Now one switches to a sum over k

$$\left[\hat{a}^j, (\hat{a}^\dagger)^j \right] = \sum_{k=0}^{j-1} \sum_{l=k}^{j-1} \binom{l}{k} \frac{j!}{(j-1-k)!} (\hat{a}^\dagger)^{j-1-k} \hat{a}^{j-1-k} \tag{16}$$

Since $\binom{b}{k} = \frac{n}{k} \binom{n-1}{k-1}$ and $\binom{0}{k} = 0$ for $k > 0$ one has that $\binom{n}{k} = 0$ for $n < k$.
Then

$$\sum_{l=k}^{j-1} \binom{l}{k} = \sum_{l=0}^{j-1} \binom{l}{k} = \binom{j}{k+1} \tag{17}$$

Finally substitution of $s := j - 1 - k$ results in

$$\left[\hat{a}^j, (\hat{a}^\dagger)^j \right] = \sum_{s=0}^{j-1} \binom{j}{j-s} \frac{j!}{s!} (\hat{a}^\dagger)^s \hat{a}^s \tag{18}$$

The next relation is $\left[\hat{n}^j, \hat{b}^\dagger \right]$. One uses again by induction.
Theorem:

$$\left[\hat{n}^j, \hat{b}^\dagger \right] = \sum_{i=0}^{j-1} (\hat{n} - 1)^i \, \hat{n}^{j-1-i} \hat{b}^\dagger. \tag{19}$$

The induction start is for $j = 1$ and reduces to $\hat{b}^\dagger$. Then

$$\left[\hat{n}^{j+1}, \hat{b}^\dagger\right] = \hat{n}^j \left[\hat{n}, \hat{b}^\dagger\right] + \left[\hat{n}^j, \hat{b}^\dagger\right] \hat{n} \tag{20}$$

$$= \hat{n}^j \hat{b}^\dagger + (\sum_{i=0}^{j-1} (\hat{n} - 1)^i \, \hat{n}^{j-1-i} \hat{b}^\dagger) \hat{n} \tag{21}$$

$$= \hat{n}^j \hat{b}^\dagger + (\sum_{i=0}^{j-1} (\hat{n} - 1)^i \, \hat{n}^{j-1-i} \left(\hat{n}\hat{b}^\dagger + \left[\hat{b}^\dagger, \hat{n}\right]\right) = \hat{n}^j \hat{b}^\dagger + \sum_{i=0}^{j-1} (\hat{n} - 1)^i \, \hat{n}^{j-1-i}(\hat{n} - 1)\hat{b}^\dagger \tag{22}$$

$$= \sum_{i=0}^{j} (\hat{n} - 1)^i \, \hat{n}^{j-i} \hat{b}^\dagger. \tag{23}$$

Now this formula can be a little bit compactified by using the binomial theorem

$$\left[\hat{n}^j, \hat{b}^\dagger\right] = \sum_{i=0}^{j-1} (\hat{n} - 1)^i \, \hat{n}^{j-1-i} \hat{b}^\dagger = \sum_{i=0}^{j-1} \sum_{s=0}^{i} \binom{i}{s} \hat{n}^s (-1)^{i-s} \hat{n}^{j-1-i} \hat{b}^\dagger \tag{24}$$

Now subsituting $k = i - s$ one reaches the formula

$$\left[\hat{n}^j, \hat{b}^\dagger\right] = \sum_{k=0}^{j-1} (-1)^k C_{jk} \hat{n}^{j-1-k} \hat{b}^\dagger, \qquad C_{jk} = \sum_{s=0}^{j-1-k} \binom{k+s}{s} = \sum_{i=0}^{j-1-k} \frac{(k+i)!}{k!}. \tag{25}$$

The next identity is $\left[\hat{n}^j \hat{b}, \hat{n}^2\right] = 2\hat{n}^{j+1}\hat{n} + \hat{n}^j \hat{b}$.

Then $\left[\hat{n}^j \hat{b}, \hat{b}^\dagger\right] = \hat{n}^j + \sum_{i=0}^{j-1} (\hat{n} - 1)^i \, \hat{n}^{j-i} = \hat{n}^j + \sum_{k=0}^{j-1} (-1)^k C_{jk} \hat{n}^{j-k}$.

It is also easy to see that $\left[\hat{n}^j, \hat{b}\right] = -\left(\left[\hat{n}^j, \hat{b}^\dagger\right]\right)^\dagger = -\sum_{i=0}^{j-1} \hat{b}\hat{n}^{j-1-i} (\hat{n} - 1)^i$.

This can also be rewritten as

$$\left[\hat{n}^j, \hat{b}\right] = -\sum_{i=0}^{j-1} (\hat{n} + 1)^i \, \hat{n}^{j-1-i} \hat{b} = -\sum_{k=0}^{j-1} C_{jk} \hat{n}^{j-1-k} \hat{b} \tag{26}$$

This then leads finally to

$$\left[\hat{n}_l^j \hat{b}_l, \hat{b}_i^\dagger \hat{b}_k\right] = \delta_{li} \left(\sum_{s=0}^{j-1} (\hat{n}_l - 1)^s \, \hat{n}_l^{j-1-s}\right) \hat{b}_i^\dagger \hat{b}_k \hat{b}_l - \delta_{lk} \hat{b}_i^\dagger \hat{b}_k \left(\sum_{s=0}^{j-1} (\hat{n}_l - 1)^s \, \hat{n}_l^{j-1-s}\right) \hat{b}_l + \delta_{li} n_l^j \hat{b}_k \tag{27}$$

$$= \delta_{li} \hat{n}_l^j \hat{b}_k + \delta_{li} \left(\sum_{s=0}^{j-1} (-1)^s C_{js} \hat{n}_l^{j-1-s}\right) \hat{n}_l \hat{b}_k - \delta_{lk} \hat{b}_i^\dagger \left(\sum_{s=0}^{j-1} C_{js} \hat{n}_l^{j-1-s}\right) \hat{b}_l^2 \tag{28}$$

Another important relation that can be easily verified is $\left[\hat{n}^m \hat{b}, \hat{n}\right] = \hat{n}^m \hat{b}$

.2 The Cumulant Expansion

The contents of this section are mostly taken from citeKubo. The Cumulant expansion is a very nice tool that can be applied to several physical problems.

Some examples are given in Kubos paper. It was one of the main tools used in this thesis.

The momentum generating function $M(\xi)$ is defined as

$$M(\xi) = \left\langle \mathrm{e}^{\xi X} \right\rangle = \sum_{n=0}^{\infty} \frac{\xi^n}{n!} \mu_n. \tag{29}$$

The cumulant function $K(\xi)$ is then given by

$$K(\xi) = \ln M(\xi) = \sum_{n=1}^{\infty} \frac{\xi^n}{n!} \kappa_n, \tag{30}$$

where κ_n is the nth cumulant and μ_n the nth moment. For N random variables $X_i, \cdots X_N$ one can defined

$$M(\vec{\xi}) \equiv \left\langle \mathrm{e}^{\vec{\xi} \cdot \vec{X}} \right\rangle = \mathrm{e}^{K(\vec{\xi})}. \tag{31}$$

$K(\vec{\xi})$ can be Taylor expanded

$$K(\vec{\xi}) = \sum_{\nu_1 \cdots \nu_N = 0}{}' \left(\prod_j \frac{\xi_j^{\nu_j}}{\nu_j!} \right) \kappa(\nu_1, \cdots, \nu_N), \tag{32}$$

where the primed summation excludes $\vec{\nu} = 0$. Further one defines the notations

$$\mu(\vec{\nu}) \equiv \left\langle X_1^{\nu_1} X_2^{\nu_2} \cdots X_N^{\nu_N} \right\rangle \tag{33}$$

$$\kappa(\vec{\nu}) \equiv \kappa(\nu_1, \cdots, \nu_N) \equiv \left\langle X_1^{\nu_1} \cdots X_N^{\nu_N} \right\rangle_c \tag{34}$$

The suffix c means cumulant or connected. The above equations define the cumulant average, e.g. $\left\langle X^2 \right\rangle_c = \left\langle X^2 \right\rangle - \left\langle X \right\rangle^2$. It is sometimes convenient to write

$$\ln \left\langle \mathrm{e}^{\vec{\xi} \cdot \vec{X}} \right\rangle = \left\langle \mathrm{e}^{\vec{\xi} \cdot \vec{X}} - 1 \right\rangle_c \tag{35}$$

Again, the suffix c denotes cumulant averaging, which by the above definitions is exactly defined for all powers of the probabilistic variables. The -1 ensures the exclusion of the $\vec{\nu} = 0$ term in the sum. A cumulant average can only be represented by lower moments, not by higher. The generalized formula is given by

$$\kappa(\vec{\nu}) = -\prod_j \nu_j! \sum_{l=1}^{n} \sum_{\{k_i\}\{m_{ij}\}: \sum_{i=1}^{l} k_i m_{ij} = \nu_j} \left(\sum_i k_i - 1 \right)! (-)^{\sum k_i} \prod_i^l \frac{1}{k_i!} \{ \frac{\mu(\vec{m}_i)}{\prod_j m_{ij}!}, \}^{k_i} \tag{36}$$

where each term corresponds to a decomposition of $n = \sum_i^N \nu_i$ objects into $\sum_i^l k_i$ subsets, which can be expressed schematically as

$$\left(X^{\nu_1} \cdots X_j^{\nu_j} \cdots X_N^{\nu_N} \right) \rightarrow \prod_{i=1}^{l} \left(X_1^{m_{i1}} \cdots X_N^{m_{Ni}} \right)^{k_i} \qquad \sum_i k_i m_{ij} = \nu_j \tag{37}$$

and

$$\mu(\vec{m}_i) = \left\langle \prod_j X_j^{m_{ij}} \right\rangle, \qquad (\vec{m}_i = (m_{i1}, \cdots, m_{iN})). \qquad (38)$$

Obviously $m_{ij} \leq \nu_j, j \in (1, \cdots, N)$, hence the cumulants are build up only with moments smaller than the ones in the cumulant.

Here are some basic theorems about cumulants:

Theorem I A cumulant $\kappa(X_1 X_1 \cdots X_n)$ is zero if one or more independent subsets of the X_i can be formed.

Corollary A cumulant is zero if one of the variables in it are zero. This is very easy to proof, since the moment generating function of the variables factors into a product and the cumulant must be a sum of the independent cumulants. So there cannot be any crossterms.

Theorem II For a stochastic variable $X(t)$ depending on a continuous parameter t one has

$$\ln \left\langle e^{\int_a^b X(t)\xi(t)dt} \right\rangle = \sum_{n=0}^{\infty} \frac{1}{n!} \int_a^b dt_1 \cdots \int_a^b dt_n \left\langle X(t_1) \cdots X(t_n) \right\rangle_c \xi(t_1) \cdots \xi(t_n)$$

$$(39)$$

$$= \sum_{n=0}^{\infty} \frac{1}{n!} \int_a^b dt_1 \int_a^{t_1} dt_2 \cdots \int_a^{t_{n-1}} dt_n \left\langle X(t_1) \cdots X(t_n) \right\rangle_c \xi(t_1) \cdots \xi(t_n)$$

$$(40)$$

Corrolary Without loss of generality one can put $\xi(t) = 1$ and obtain

$$\ln \left\langle e^{\int_a^b X(t)dt} \right\rangle = \sum_{n=0}^{\infty} \frac{1}{n!} \int_a^b dt_1 \cdots \int_a^b dt_n \left\langle X(t_1) \cdots X(t_n) \right\rangle_c \qquad (41)$$

$$= \sum_{n=0}^{\infty} \int_a^b dt_1 \int_a^{t_1} dt_2 \cdots \int_a^{t_{n-1}} dt_n \left\langle X(t_1) \cdots X(t_n) \right\rangle_c \qquad (42)$$

Also

$$\ln \left\langle e^{\int_a^b X(t)dt} \right\rangle = \left\langle e^{\int_a^b X(t)dt} - 1 \right\rangle_c \qquad (43)$$

Those equations can be generalized to include vectors of random variables $\vec{X}$

$$\ln \left\langle e^{\int_a^b \sum_j X_j(t)dt} \right\rangle = \sum_{n=1}^{\infty} \frac{1}{n!} \int_a^b dt_1 \cdots \int_a^b dt_n \sum_{j_1} \cdots \sum_{j_n} \left\langle X_{j_1} \cdots X_{j_n} \right\rangle_c \qquad (44)$$

and to continuous variables

$$\ln \left\langle e^{\int \int X(s,t)\,ds\,dt} \right\rangle = \sum_{n=1}^{\infty} \frac{1}{n!} \int ds_1 \cdots \int ds_n \int dt_1 \int dt_n \left\langle X(s_1 t_1) \cdots X(s_n t_n) \right\rangle_c$$

$$(45)$$

For a proof of this theorem, one rewrites the integration as a sum over many

small intevals with the new set of variables $X(t_i)\delta t_i$. But for $\delta t \to 0$, only cumulants with $\nu_i \neq 1$ remain, since

$$\lim \sum_j \left\langle X(t_j)^2 \right\rangle_c (\delta t_j)^2 = \lim O(\delta t) \times \int_a^b \left\langle X^2(t) \right\rangle_c dt = 0. \qquad (46)$$

Cluster Expansion

The cumulant can be expanded in cluster

$$K(\vec{\xi}) = \sum{}' \prod_i \frac{\xi_i^{\nu_i}}{\nu_i!} \kappa(\vec{\nu}) = \sum_l K_l \qquad (47)$$

Starting point is the set of cumulants $K_1(X_i)$ which contain a particular variable X_i

$$M_1(X_i) \equiv \left\langle e^{\xi_i X_i} \right\rangle = e^{K_1(X_i)} \qquad (48)$$

So

$$K_1 = \sum_i K_1(X_i). \qquad (49)$$

The next term is of the form

$$K_2 = \sum_{(i,j)} K_2(X_i, X_j). \qquad (50)$$

K_2 contains all term with two variables X_i, X_j in the cumulant series.

$$e^{K_2(X_i,X_j)} = \frac{M_2(X_i, X_j)}{M_1(X_i)M_2(X_j)}. \qquad (51)$$

One then proceeds to expanded

$$K = \sum_{n=1}^N \sum_{\{n\}_N} K_n(\{n\}_N), \qquad (52)$$

where the function $K_n(\{n\}_N)$ contains any of the variables

$$\{n\}_N \equiv (X_{i_1}, \cdots X_{i_n}) \qquad (53)$$

at least once. One can use the same arrangement principles for a hierarchy of functions $U_n(\{n\}_N)$, depending on sets of n variables out of a given set of N variables.

$$\{n\}_N = (X_{i_1} \cdots X_{i_n}) \text{ selected from } \{N\} = (X_1, \cdots X_N) \qquad (54)$$

The nth moment generating function can then be defined

$$M_n(\{n\}_n) = \left\langle \exp U_n \left(\{n\}_N\right) \right\rangle. \qquad (55)$$

Then the functions $K_n \left(\{n\}_N\right)$ can be introduced and the cumulant function $K(\{N\})$ can be defined as

$$M(\{N\}) \equiv \left\langle e^{U(\{N\})} \right\rangle = e^{K(\{N\})}. \qquad (56)$$

So

$$K(N) = \sum_n K_n = \sum_n \sum_{\{n\}_N} K_n(\{n\}_N). \tag{57}$$

Theorem III: In the cluster expansion of the cumulant function $K(\{n\})$, the cluster cumulant function $K_n(\{n\}_N)$ for a set of n variables is given explicitly by

$$K_n(\{n\}_N) = \sum_{l=1}^n (-)^{n-l} \sum_{\{l\}_n} \ln M_l(\{l\}_N) \tag{58}$$

or

$$\mathrm{e}^{K_n(\{n\}_N)} = \frac{M_n(\{n\}_N) \prod M_{n-2}(\{n-2\}_N) \cdot \cdots \cdot \prod M_2(i,j)}{\prod M_{n-1}(\{n-1\}_N) \prod M_{n-3}(\{n-3\}_N) \cdots \prod M_1(i)} \tag{59}$$

if n is even.

$$\mathrm{e}^{K_n(\{n\}_N)} = M_n(\{n\}_N) \frac{\prod M_{n-2}(\{n-2\}_N) \cdots \prod M_1(i)}{\prod M_{n-1}(\{n-1\}_N) \cdots \prod M_2(i,j)} \tag{60}$$

if n is odd.

Theorem IV: If the set $\{n\}_N$ is divided into independent sets $\{n'\}_N$ and $\{n''\}_N$, namely if

$$\{n\}_N = \{n'\}_N + \{n''\}_N \tag{61}$$

and

$$M(\{n\}_N) = M(\{n'\}_N) \times M(\{n''\}_N). \tag{62}$$

then

$$K_n(\{n\}_N) = \equiv K_{n'+n''}(\{n'+n''\}_N) = 0, \tag{63}$$

and more generalls

$$K_{m'+m''}(\{m'\}_{n'} + (\{m''\}_{n''}) = 0 \tag{64}$$

if neither $\{m'\}$ nor $\{m''\}$ is empty.

This way one can define connected sets and connected cumulant functions, by requiring that the combined cumulant function is non-zero.

Generalized Exponential Functions

A generalized exponential can be defined for variables, that are not necessarily c-numbers. One has to introduce an additional ordering O such that

$$\mathrm{e}^{x+y} \equiv \mathrm{e}_O^{x+y} \equiv O\left(\mathrm{e}^{x+y}\right) = O\left(\mathrm{e}^x \cdot \mathrm{e}^y\right). \tag{65}$$

There are many ways to generalize exponentials by defining different prescriptions.

Generalized Moments, Cumulants and Cumulant Functions

One can define a generalized average operation A for variables $(X_1, \ldots, X_N)$ such that moments and moment generating functions are convergent

$$A(\mathrm{e}^{\sum_i \xi_i X_i}) \equiv \left\langle \mathrm{e}^{\sum_i \xi_i X_i} \right\rangle = \sum_{\nu_1=0}^\infty \cdots \sum_{\nu_N=0}^\infty \prod \frac{\xi_i^{\nu_i}}{\nu_i!} A\left(X_1^{\nu_1} \ldots X_N^{\nu_N}\right). \tag{66}$$

The averaged is assumed to satisfy the normalization condition

$$A(1) = 1. \tag{67}$$

Sometimes the average is still a q-number. Then the normalization is required to give the identity in the field of q-numbers. The exponential function with respect to an ordering Q is defined as

$$\mathrm{e}_Q^{\sum_i \xi_i X_i} \equiv Q\mathrm{e}^{\sum_i \xi_i X_i}. \tag{68}$$

Then one can redefine

$$\left\langle \mathrm{e}_Q^{\sum_i \xi_i X_i} \right\rangle = \mathrm{e}_Q^{K(\xi_1,\ldots,\xi_N)} \tag{69}$$

The generalized moments are then defined by

$$\mu(\nu_1,\ldots,\nu_N) = A\left(Q\prod X_i^{\nu_i}\right). \tag{70}$$

If the cumulants are not c-numbers, then one has to have an ordering in the exponential for

$$\exp_Q \sideset{}{'}\sum_{\nu_1\ldots\nu_N} \prod \frac{\xi_i^{\nu_i}}{\nu_i!}\kappa(\vec{\nu}) \equiv \sum_{n=0} \frac{1}{n!}Q\{\sideset{}{'}\sum\prod \frac{\xi_i^{\nu_i}}{\nu_i!}\kappa(\vec{\nu})\}^n = \sum_{\nu_1\ldots\nu_N}\prod \frac{\xi_i^{nu_i}}{\nu_i!}\mu(\vec{\nu}) \tag{71}$$

Theorem V: Theorem I-IV are valid for the generalization to q-numbers from c-numbers.

This means

$$\left\langle \exp_Q \sum_i \xi_i X_i \right\rangle = \exp_Q \left\langle \mathrm{e}_Q^{\sum_i \xi_i X_i} - 1 \right\rangle_c \tag{72}$$

and

$$\left\langle Q\prod_j X_j^{\nu_j} \right\rangle_c = -\prod \nu_j! \sum_{l=1}^n \sum_{\sum_{i=1}^l k_i m_{ij}=\nu_j} \left(\sum_i k_i - 1\right)!(-)^{\sum_i k_i} \tag{73}$$

$$\times Q\prod_{i=1}^l \frac{1}{k_i!}\{\frac{\left\langle Q\prod X_j^{m_{ij}}\right\rangle}{\prod m_{ij}!}\}^{k_i} \tag{74}$$

If one has after the average not a c-number, but a q-number to be ordered, one can find that if $X(t) = Y(t)Z(t)$ and the ordering can be separated into $O = O_z O_y$, where the average is only defined for the Ys, then

$$\left\langle \exp_O\{\int_0^t Y(t')Z(t')dt'\} \right\rangle = \exp_{O_z} \left\langle \exp_O\left(\int_0^t Y(t')Z(t')dt'\right) - 1 \right\rangle_c = \exp_{O_z} K(t) \tag{75}$$

The cumulant expansion for Hubbard operators

One can use the cumulant expansion to evaluate averages of diagonal Hubbard operators. The exponential can be cumulant expanded to

$$\left\langle \exp\left(\sum_i \eta_i X^{\alpha_i}\right) \right\rangle_0 = \exp\{\sum_{n=1}^\infty \frac{1}{n!}\sum_{i_1}\cdots\sum_{i_n}\eta_{i_1}\ldots\eta_{i_n}\left\langle X_{i_1}\cdots X_{i_n}\right\rangle_c\}. \tag{76}$$

The solutions are for example of the form

$$\left\langle (X^{p_1 p_1})^2 X^{p_2 p_2} \right\rangle = (b^{p_1})^2 b^{p_2} + b^{p_1 1 p_1} b^{p_2} + 2 b^{p_1 p_2} b^{p_1} + b^{p_1 p_1 p_2} \tag{77}$$

with

$$b^{p_i} = \left\langle X^{p_i p_i} \right\rangle_0 = \frac{e^{-\beta \lambda_i}}{\sum_k e^{-\beta \lambda_k}} \tag{78}$$

$$b^{p_i p_k} = \left\langle X^{p_i p_i} X^{p_k p_k} \right\rangle_{0c} = \frac{\partial}{\partial(-\beta \lambda_k)} b_{p_i} \tag{79}$$

$$b^{p_i p_k p_n} = \left\langle X^{p_i p_i} X^{p_k p_k} X^{p_n p_n} \right\rangle_{0c} = \frac{\partial^2}{\partial(-\beta \lambda_k)\,\partial(-\beta \lambda_n)} b_{p_i} \tag{80}$$

One can easily show, that the last formulas must be correct. For the zeroth approximation one can find the generating function

$$Z(\vec{\xi}) = \frac{\mathrm{Tr}\left(e^{\sum_i (-\beta \lambda_i + \xi_i) X^{ii}}\right)}{Tr\left(e^{\sum_i \lambda_i X^{ii}}\right)} = \frac{\sum_i e^{-\beta \lambda_i + \xi_i}}{\sum_i e^{-\beta \lambda_i}} \tag{81}$$

From equation (3.81) it is clear, that the moments are invariant under permutation (Schwarz theorem/theorem of symmetry of derivatives). Because of that and general formula(see appendix), which relates the cumulants to the moments, all cumulants with the same groups of indices ν are the same. From equation (76) follows then, that

$$\left\langle X_1^{\nu_1} \dots X_n^{\nu_n} \right\rangle_c = \frac{\partial^{\nu_1}}{\partial \xi_1^{\nu_1}} \cdots \frac{\partial^{\nu_n}}{\partial \xi_n^{\nu_n}} \ln Z(\vec{\xi})\Big|_{\vec{\xi} \to 0}. \tag{82}$$

The factor of $n!$ cancels, because there are $\frac{n!}{\prod \nu_i!}$ terms of equal contribution. Further

$$\frac{\partial^{\nu_i}}{\partial \xi_i^{\nu_i}} \xi_i^{\nu_i} = \nu_i!, \tag{83}$$

so those tems cancel too. Since $\ln Z = \ln \sum_i e^{-\beta \lambda_i + \xi_i} + const.$ Performing the differentiation and taking the limit of $\vec{\xi} \to 0$ one arrives at

$$\left\langle X_1^{\nu_1} \dots X_n^{\nu_n} \right\rangle_c = \sum_{i_1=1}^{\nu_1} \cdots \sum_{i_n=1}^{\nu_n} (-1)^{\sum_k i_k - 1} (\sum_k i_k - 1)! \frac{e^{-\beta \sum_k i_k \lambda_k}}{\left(\sum_i e^{-\beta \lambda_i}\right)^{\sum i_k}} \tag{84}$$

This is indeed the same as

$$\left(\prod_{i=2}^{n} \frac{\partial^{\nu_i}}{\partial(-\beta \lambda_i)^{\nu_i}} \right) \frac{\partial^{\nu_1 - 1}}{\partial(-\beta \lambda_1)^{\nu_1 - 1}} \frac{e^{-\beta \lambda_1}}{\sum_j e^{-\beta \lambda_j}} \tag{85}$$

Now in equation (76) appears a sum over all possible cumulant combinations of the $\sum_i \nu_i$ elements. The symmetry factor of an arbitrary group

$$\left\langle X_1^{\nu_{11}} \dots X_n^{\nu_{n1}} \right\rangle_c^{N_1} \dots \left\langle X_1^{\nu_{1M}} \dots X_n^{\nu_{nM}} \right\rangle_c^{N_M} \tag{86}$$

is given by

$$\frac{\prod_i (\sum_j \nu_{ij} N_j)!}{\prod_i \prod_j (\nu_{ij}!)^{N_k} \prod_k N_k!} \tag{87}$$

This can be easily generalized by adding indices for different groups, which would just be another effective index ν'_{ii}. According to theorem I , the cumulants of mixtures of independent groups are zero, so one has in general fewer terms to consider.

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Selbstständigkeitserklärung

Hiermit erkläre ich die vorgelegte Arbeit selbst verfasst und keine anderen als die angegebenen Quellen und Hilfsmittel verwendet zu haben.

München, den 09.09.2012

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