Emergent Phenomena in Quantum Critical Systems

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EMERGENT PHENOMENA IN QUANTUM CRITICAL SYSTEMS

A Dissertation Presented
by
KUN CHEN

Submitted to the Graduate School of the University of Massachusetts Amherst in partial fulfillment of the requirements for the degree of

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Department of Physics
EMERGENT PHENOMENA IN QUANTUM CRITICAL SYSTEMS

A Dissertation Presented

by

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A quantum critical point (QCP) is a point in the phase diagram of quantum matter where a continuous phase transition takes place at zero temperature. Low-dimensional quantum critical systems are strongly correlated, therefore hosting nontrivial emergent phenomena.

In this thesis, we first address two decades-old problems on quantum critical dynamics. We then reveal two novel emergent phenomena of quantum critical impurity problems.

In the first part of the thesis, we address the linear response dynamics of the (2 + 1)-dimensional $O(2)$ quantum critical universality class, which can be realized in the ultracold bosonic system near the superfluid (SF) to Mott insulator (MI) transition in two dimensions. The first problem we address is about the fate of the massive Goldstone (Higgs) mode in the two-dimensional relativistic theory. Using large-scale Monte Carlo simulations and numerical analytical continuation, we obtain universal spectral functions in SF, MI and normal quantum critical liquid phases and reveal that they all have a relatively sharp resonant
peak before saturating to the critical plateau behavior at higher frequencies. The universal resonance peak in SF reveals a critically-defined massive Goldstone boson, while the peaks in the last two phases are beyond the predictions of previous theories. The second problem we address is to controllably calculate one of the most fundamental transport properties—optical conductivity—in the quantum critical region. We precisely determine the conductivity on the quantum critical plateau, $\sigma(\infty) = 0.359(4)\sigma_Q$ with $\sigma_Q$ the conductivity quantum. For the first time, the shape of the $\sigma(i\omega_n) - \sigma(\infty)$ function in the Matsubara representation is accurate enough to compare a holographic gauge-gravity duality theory for transport properties [Myers, Sachdev, and Singh, Phys. Rev. D 83, 066017 (2011)] to the reality. We find that the theory—in the original form—can not account for our data, thereby inspiring the theorists to modify the corresponding holographic theory.

The second part of this thesis discusses two exotic impurity states hosted by quantum critical environments. The first one is the halon, a novel critical state of an impurity in $O(N \geq 2)$ quantum critical environment. We find that varying the impurity-environment interaction leads to a boundary quantum critical point (BQCP) between two competing ground states with charges differing by $\pm 1$. In the vicinity of the BQCP, the halon phenomenon emerges. The hallmark of the halon physics is that a well-defined integer charge carried by the impurity gets fractionalized into two parts: a microscopic core with half-integer charge and a critically large halo carrying a complementary charge of $\pm 1/2$. The halon can be generalized to other incompressible quantum-critical environments with particle-hole symmetry.

The second novel phenomenon we reveal is termed ”trapping collapse”. We address a simple fundamental question of how many repulsively interacting bosons can be localized by a trapping potential. We find that under rather generic conditions, for both weakly and strongly repulsive particles, in two and three dimensions—but not in one-dimension!—this potential well can trap infinitely many bosons. Even hard-core repulsive interactions do not
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INTRODUCTION

In many-body systems, particles may cooperate through interactions, giving rise to a macroscopic collective state governed by a set of new physical laws that are very different from the microscopic equations of motion. These new physical laws describe collective degrees of freedom rather than underlying particles, thus overriding the relevance of microscopic details. This concept is known as emergence. It can bridge the atomic scales to the macroscopic scales of quantum matter, therefore playing a vital role in condensed matter physics.

The best known example of emergence is the ordering caused by spontaneous symmetry breaking: to minimize free energy, a macroscopic system may have to break the symmetry of microscopic equations of motion. As a result, it transitions into a phase with long-range order. Taking an interacting bosonic gas as an example, when the system breaks the global $U(1)$ symmetry, it will turn into a superfluid. Although the superfluid consists of quantum particles, its emergent physics has purely classical nature, which is the Hamiltonian mechanics of a complex scalar field [6].

A very special type of emergence can be found on the approach to a continuous phase transition. The point at which the transition happens is called a critical point. Even though on the verge of entering a symmetry-breaking phase, the system right at the critical point actually has higher symmetry than that of the microscopic equations. Indeed, it gains an emergent symmetry known as scale invariance, namely the effective field theory does not vary if length (and time) scales are redefined. Though critical points are ubiquitous in nature, there are relatively few scale-invariant field theories. The solution to this paradox resides in the physics of universality near critical points: many-body systems may have various scale-
dependent microscopic details, but these details play progressively less important role as the phase transition is approached. Eventually, at the critical point, many systems end up with the same predominating universal physics described by a scale-invariant field theory.

In this prospectus, we will focus on the emergent phenomena in quantum critical systems described by a simple but fundamentally important continuous field theory, the $O(N)$-symmetric $\Psi^4$ model,

$$Z = \int \mathcal{D}\Psi(r, \tau) e^{-S_{\text{eff}}},$$

$$S_{\text{eff}} = \int_0^{\beta} d\tau \int d^d r \left[ \frac{1}{2} \left| \frac{\partial \Psi}{\partial \tau} \right|^2 + \frac{1}{2} |\nabla \Psi|^2 + \frac{g}{2} |\Psi|^2 + \frac{u}{4} |\Psi|^4 \right].$$

Here $\Psi$ is the $N$-component continuous vector field, $g$ is the control parameter and $u$ is the interaction strength which is positively defined so that the action is bounded from below. This model is defined in the manifold of $d \geq 2$ spatial dimensions and one imaginary-time dimension. The total length of the time coordinate $\beta = 1/T$ is the inverse temperature of the underlying quantum system, and periodic boundary conditions are imposed along the time coordinate. The imaginary time is actually a mathematical dimension arising from the path integral representation for the partition sum of a quantum system in thermal equilibrium[6]. Therefore, it should not be confused with the physical time of the microscopic equations of motion. Still, imaginary-time correlation functions encode complete information of the corresponding real-time linear response functions. Therefore, not only the static properties but also the linear response dynamics of the quantum system are effectively captured by the $\Psi^4$ model.

At zero temperature, the spatial and the imaginary-time dimensions form a $(d + 1)$-dimensional manifold so that the $\Psi^4$ model gains space-time symmetry. This observation immediately implies that the long-wavelength dynamics of the underlying quantum system are Lorentz invariant! In other words, the system hosts an emergent relativistic “universe”,

2
where there is an effective speed limit well below the speed of light. The collective modes living in this “universe” are all bounded by this speed limit.

The \( \Psi^4 \) model describes many physical systems in condensed matter. The \( O(2) \) \( \Psi^4 \) theory is the effective model of interacting bosons in an external commensurate potential near the superfluid (SF) to Mott insulator (MI) quantum phase transition with particle-hole symmetry. In this theory, \( \Psi \) is the coarse-grained field of the bosonic annihilation operator. The \( O(3) \)-symmetric \( \Psi^4 \) model describes “dimerized” antiferromagnets in which each unit cell contains even number of spins. In this case, \( \Psi \) is the coarse-grained field of the local staggered magnetization.

![Figure 1. Schematic phase diagram of the \( \Psi^4 \) model in the parameter space spanned by temperature \( T \) and control parameter \( g \). The quantum critical point \( g_c \) controls the low-temperature physics of the system in a wide parameter range.](image)

The phase diagram of the \( \Psi^4 \) model is shown in Fig. 1. At low temperature, the system undergoes a continuous phase transition from the disordered phase into an ordered phase that breaks the \( O(N) \) symmetry. The phase transition at finite temperature is qualita-
tively different from that at absolute zero temperature. The finite-temperature transition is driven by thermal fluctuations and only spatial length scale diverges, therefore its criticality is described by a $d$-dimensional classical scale-invariant theory. On the other hand, the zero-temperature phase transition is driven by quantum fluctuations, therefore featuring a quantum critical point (QCP). At this QCP, both spatial and temporal characteristic length scales diverge, leading to a $(d+1)$-dimensional scale-invariant field theory with “relativistic” dynamics.

The quantum criticality controls the low-temperature physics near the QCP. At nonzero temperature, thermal fluctuations with an energy scale of $k_B T$ compete with the quantum fluctuations at the characteristic energy scale $\Delta$, where $\Delta$ is the characteristic energy. The region $\Delta > k_B T$ is known as a quantum critical region, where the subtle interplay between thermal and quantum fluctuations gives rise to nontrivial physics.

Among the fundamental problems of quantum criticality is the universal linear response dynamics, which includes experimentally observable spectral functions and transport properties. To understand the dynamics, it is important to reveal the properties of all well-defined collective modes in the system. The situation becomes particularly intriguing near the QCP in low dimensions. Since the critical system is strongly coupled in this case, a simple description in terms of weakly interacting collective modes is uncontrolled and perturbation theories fail even qualitatively. This is exactly what happens in the vicinity of the $(2 + 1)$-dimensional $O(N)$ QCP. Though it is considered to be one of the best studied strongly interacting systems, its quantum critical dynamics is still poorly understood, both theoretically and experimentally. In the first part of the thesis, we address two decades-old problems on the quantum critical dynamics.

We first study the properties of collective modes near the two-dimensional superfluid (SF) to Mott insulator (MI) quantum phase transition at constant density [7, 8], which is described by the $(2 + 1)$-dimensional $O(2)$ universality class. We calculate the spectral function for
the magnitude squared of the order parameter. The universal functions for the superfluid, Mott insulator, and normal liquid in the quantum critical region reveal a massive Goldstone (Higgs) resonance [9] which is relatively sharp and is followed by a damped oscillation (in the first two phases only) before saturating to the quantum critical plateau. In order to understand the counter-intuitive massive Goldstone resonance in the insulating and normal phases, we propose a picture of a scale-dependent Mexican hat.

We then study the universal quantum transport in the quantum critical regime of the (2 + 1)-dimensional $O(2)$ universality class [10]. Based on large-scale Monte Carlo simulations of the classical (2 + 1)-dimensional $J$-current model and the two-dimensional Bose-Hubbard model, we can precisely determine the conductivity on the quantum critical plateau, $\sigma(\infty) = 0.359(4)\sigma_Q$ with $\sigma_Q$ the conductivity quantum. According to a recent theory [11], the universal conductivity is an example where the anti-de Sitter/conformal field theory (AdS/CFT) correspondence from string theory can be used. The theory utilizes the conjecture that a strongly interacting quantum critical theory can be mapped to a weakly interacting quantum gravity theory in a anti-de Sitter space, where the transport is then perturbatively calculated. In our calculation, the shape of $\sigma(i\omega_n) - \sigma(\infty)$ function in the Matsubara representation is accurate enough to conclusively test the theory. We find that it can not fit the data unless the temperature of the horizon of the black hole in the gravity theory is different from the temperature of the conformal field theory. Our result has inspired theorists to find a new holographic theory [12], which introduces a new relevant term in the quantum gravity theory and turns out to be compatible with our data.

Another kind of fundamental problems of quantum criticality is the critical impurity problems. Due to the strong interaction in the quantum critical system, even the simplest impurity problem, namely a trapping potential (or a potential bump) coupled to the charge density of the environment, becomes highly nontrivial. Many questions of fundamental importance have not yet been addressed. In the second part of the this thesis, we address
two of them: Is the effective charge of the impurity still quantized or not? And if not, is the
effective charge always bounded from above?

We investigate the impurity charge quantization in different quantum critical systems. We find that an impurity in a two-dimensional $O(N)$ quantum critical environment can get
dressed into a special critical state, which we term the halon [13]. The hallmark of the halon
physics is that a well-defined integer impurity charge gets fractionalized into two parts: a mi-
icroscopic core with half-integer charge and a critically large halo carrying a complementary
charge of $\pm 1/2$. The halon phenomenon emerges when the impurity–environment interac-
tion is fine-tuned to the vicinity of a boundary quantum critical point (BQCP), at which the
energies of two quasiparticle states with adjacent integer charges approach each other. The
universality class of such BQCP is captured by a model of pseudo-spin-1/2 impurity coupled
to the quantum-critical environment, in such a way that the rotational symmetry in the
pseudo-spin $xy$-plane is respected, with a small local “magnetic” field along the pseudo-spin
$z$-axis playing the role of control parameter driving the system away from the BQCP. On
the approach to BQCP, the half-integer projection of the pseudo-spin on its $z$-axis gets de-
localized into a halo of critically divergent radius, capturing the essence of the phenomenon
of charge fractionalization. With large-scale Monte Carlo simulations, we confirm the exis-
tence of halons—and quantify their universal features—in $O(2)$ and $O(3)$ quantum critical
systems.

To answer the second question about the existence of the upper bound for the effec-
tive charge, we find counterexamples where the impurity charge actually diverges in bosonic
systems with ill-defined compressibility (say, a quantum critical system right at the vacuum-
superfluid or at a generic superfluid–Mott-insulator phase transition point) [14]. We term
this effect the “trapping collapse”. It is related to a simple fundamental question we have
addressed: how many repulsively interacting bosons can be localized by trapping potentials.
We find that under rather generic conditions, for both weakly and strongly repulsive parti-
cles, in two and three dimensions—but not in one-dimension!—the potential well can trap infinitely many bosons. For example, even hard-core repulsive interactions do not prevent the trapping collapse phenomenon from taking place. For the weakly interacting/dilute regime, the effect can be revealed by the mean-field argument, while in the case of strong correlations the evidence comes from path-integral simulations. We also discuss the possibility of having a transition between the infinite and finite number of trapped bosons when strong repulsive inter-particle correlations are increased.

The thesis is organized as follows. In Chapter 1, we introduce the models and numerical methods used in our study. Then we move to the first part of the thesis about quantum critical dynamics. Chapter 2 discusses the universal behavior of the massive Goldstone mode in the vicinity of the QCP. In Chapter 3, we provide the detailed experimental conditions to observe this mode. In Chapter 4, we further discuss universal conductivity in the quantum critical regime, then use our calculations to test a holographic theory. Starting from Chapter 5, we discuss the impurity problem in quantum critical systems. We first explain the setup of the impurity problem in Chapter 5. Then we describe the halon physics in Chapter 6 and introduce the trapping collapse effect in Chapter 7.
CHAPTER 1
MICROSCOPIC MODELS AND NUMERICAL METHODS

Ultracold bosons in optical lattices offer unique possibilities to study the two dimensional superfluid (SF) to Mott insulator (MI) quantum phase transition [15, 16], which is a QCP of the (2+1)-dimensional $O(2)$ universality class. At low enough temperatures the physics of the system can be described by the Bose-Hubbard (BH) model [17, 18], which is parametrized by a hopping amplitude $J$ and an on-site interaction energy $U$,

$$\hat{H}_0 = -J \sum_{\langle i,j \rangle} (b_i^\dagger b_j + H.c.) + \frac{U}{2} \sum_i n_i(n_i - 1) - \mu \sum_i n_i,$$  \hspace{1cm}(1.1)$$

where $b_i^\dagger$ ($b_i$) creates (annihilates) a particle on the site $i$, and $\langle i,j \rangle$ denotes the sum over nearest neighbors on the square lattice. The phase diagram of the two dimensional Bose-Hubbard model and its phase diagram shown in Fig. 1 is known with high accuracy [19, 2, 20] at both zero and finite temperature. In the ground state, the system undergoes a continuous phase transition from the superfluid (SF) to the Mott insulator (MI) when decreasing the ratio $j = J/U$ at fixed integer filling factor (at the tip of each lobe in the phase diagram 1). At filling factor $\langle n \rangle = 1$, the transition occurs at $j_e^{-1} = 16.7424(1)$ and $\mu_e/J = 6.21(2)$ and features a (2 + 1)-dimensional $O(2)$ QCP.

This QCP can also be studied with classical models. One of the simplest choices is the three-dimensional classical J-current model with $L^2 \times L_z$ sites [21],

$$H = \frac{1}{2K} \sum_{\langle ij \rangle} J_{<ij>}^2,$$ \hspace{1cm}(1.2)$$
Figure 1.1. Schematic zero-temperature phase diagram of the Bose Hubbard model in the parameter space spanned by the chemical potential $\mu$ and the hopping amplitude $J$.

where $J_{ij} \in (-\infty, \infty)$ are integer valued bond currents between the neighboring sites subject to the zero-divergence constraint such that the allowed configurations form closed loops. The continuous phase transition point is located at $K_c = 0.3330670(2)$ [10].

Similar to the J current model, the configuration space of the Bose Hubbard model partition sum also consists of closed (particle/hole) loops in the Fock state path integral formalism, as shown in Fig. 1.2. Therefore, both the classical and quantum model can be efficient sampled with a similar Monte Carlo method with worm algorithm [22, 23, 24]. Rather than the partition sum with closed-loop configurations, worm algorithm samples Green’s function, which enlarges the partition sum configurations with two additional open legs as shown in Fig. 1.3.
Figure 1.2. Left: A path integral configuration for the partition sum of the Bose Hubbard model defined on a periodic lattice chain. At a given time slice, the dashed line represents a zero-occupancy state, the solid line (the world line) represents state with occupation number $\geq 1$. The configuration satisfy the periodic condition along the imaginary-time direction. As a result, the world line of any particle forms a closed loop. Right: A possible Monte Carlo move to update the partition-function configurations. The blue solid line represents a world line of a particle. After the update, a local part of the world line is replaced with a new trajectory. Being local, such updates can not change the topology of the world line.

The algorithm utilizes the fact that Green’s function is proportional to the partition sum when its two external legs are closed. Therefore, by randomly shuffling these external legs in space-time, the algorithm samples not only the full Green’s function but also the partition sum as a by-product. It nearly eliminates critical slowing down therefore can be highly efficient near the critical point.

The Monte Carlo simulations does not provide direct access to linear response dynamics. To calculate the dynamics, a technique known as numerical analytical continuation is required. This technique utilizes the Kramers-Kröning relation which relates the imaginary part of any (two point) response function in real frequency, $\text{Im}\chi(\omega)$, to a (two point) correlation function in Matsubara frequency, $\chi(i\omega_n)$,

$$\chi(i\omega_n) = \int_0^{+\infty} \frac{d\omega}{\pi} \frac{2\omega}{\omega^2 + \omega_n^2} \text{Im}\chi(\omega)$$

(1.3)

In simulation, the Matsubara frequency correlation function $\chi(i\omega_n)$, or its Fourier transformation $\chi(\tau)$, can be directly measured. Then an inverse transform, which is exponentially
Figure 1.3. Left: A path integral configuration for the Green’s function of the Bose Hubbard model defined on a periodic lattice chain. The configuration consists of two additional open legs. The leg associated with the creation operator is illustrating Masha (M) and the one with the annihilation operator is Ira (I). Right: A schematic cartoon to show the worm algorithm. The blue solid line is the world line connecting two legs. The algorithm opens a closed world line with two legs, then allows Ira to perform a random walk on the spacetime torus until it meets Masha. Although each update is still local, the topology of a world line can be changed by the above steps. At each time when Ira and Masha meet, a partition-function configuration is created.

Sensitive to this measurement, is required to obtain the real frequency dynamics. Because of the presence of statistical noise in $\chi(i\omega_n)$, the problem is ill-defined. In practice, a carefully designed smoothening protocol can be used to acquire a physically acceptable solution. A detailed discussion of the protocol used in our studies can be found in Ref. [5].
Part I
Quantum Critical Dynamics
CHAPTER 2
FATE OF THE MASSIVE GOLDSTONE MODE NEAR QUANTUM CRITICALITY

The text of this chapter has been adapted from Ref. [7].

2.1 Introduction

Collective modes are important for understanding dynamic susceptibilities, which include experimentally observed spectral functions and transport properties. The situation becomes particularly intriguing in strongly coupled systems, where a simple description in terms of weakly interacting excitations is unreliable and perturbation theories fail even qualitatively. Under these conditions, the role of underlying collective modes on dynamic susceptibilities becomes increasingly more important but is hard to calculate [25]. This is exactly what happens in the vicinity of the two-dimensional (2D) superfluid-to-Mott insulator quantum critical point (SF-MI QCP) [17]. Though it is considered to be one of the best studied strongly coupled systems, its quantum critical dynamics is still poorly understood, both theoretically and experimentally.

In superfluids near SF-MI quantum criticality, the effective field theory in terms of a complex scalar order parameter \( \Psi \) features an emergent particle-hole symmetry and Lorentz invariance, and is expected to have two types of collective modes. [9] The first one originates from fluctuations of the phase of \( \Psi \) and describes a massless Bogoliubov-Nambu-Goldstone mode. The second one describes amplitude fluctuations and is associated with a massive
Goldstone (MG) mode[9]. The fate of the MG-mode in 2D is an intriguing and controversial issue because its decay into lower-energy gapless modes is found to be strong.

Mean-field theory predicts a stable massive Goldstone particle. In (3 + 1) dimensions, where the QCP is a Gaussian fixed point (with logarithmic UV corrections), there is compelling experimental evidence for the existence of a massive Goldstone mode, most beautifully illustrated for the TlCuCl$_3$ compound [26]. In (2 + 1) dimensions, where scaling theory is expected to apply, the massive Goldstone particle is strongly coupled to sound modes and it was argued for a long time, on the basis of a $1/N$-expansion to leading order ($N = 2$ corresponds to our case), that it cannot survive near criticality [27, 28, 29, 25]. Moreover, since the longitudinal susceptibility diagram has an IR divergence going as $\omega^{-1}$, it may well dominate any possible massive Goldstone peak. However, it was recently emphasized that the type of the probe is important [30, 31, 32]: for scalar susceptibility (i.e., the correlation function of $|\psi|^2$) the spectral function $S(\omega)$ vanishes as $\omega^3$ at low-frequencies [27, 30], and this offers better conditions for revealing the massive Goldstone peak.

Recently, the cold atom experiment [3], where a 2D Bose-Hubbard system was gently “shaken” by modulating the lattice laser intensity and probed by in-situ single site density measurements, saw a broad spectral response whose onset softened on approach to the QCP, in line with the scaling law (2.1), however no massive Goldstone resonance is found. This outcome can be explained by tight confinement, finite temperature, and detuning from the QCP, as shown by our recent Quantum Monte Carlo (MC) simulations [1] performed for the experimental setup ‘as is’ in the spirit of the quantum simulation paradigm [33]. On the other hand, simulations for the homogeneous Bose-Hubbard model in the vicinity of the SF-MI point featuring emergent particle-hole symmetry and Lorentz-invariance [17] unambiguously revealed a well-defined massive Goldstone resonance which becomes more pronounced on approach to the QCP [1].
However, the universal structure of the spectral function $S(\omega)$ is beyond the reach of previous studies [3, 1, 34]. In the scaling limit, the theory predicts that $S(\omega)$ in the vicinity of QCP takes the form

$$S(\omega) \propto \Delta^{3-2/\nu} \Phi\left(\frac{\omega}{\Delta}\right),$$

which valids not only in the SF phase but also in the MI phase and normal liquid phase in the quantum critical regime (NL). $\Delta$ is characteristic energy in each phase (massive Goldstone mass for SF, Mott gap for MI and temperature for NL), and $\nu = 0.6717$ is the correlation length exponent for the $U(1) \equiv O(2)$ universality in $(2 + 1)$ dimensions [4, 35]. Despite that the universal functions $\Phi(x)$ are different in three phases, all of them are expected to saturate to the same quasi plateau $\Phi(x \gg 1) \propto x^{3-2/\nu} \approx x^{0.0225}$. This plateau is a crucial ingredient of the universal physics, which is clearly absent in previous studies of the SF phase [3, 1].

The massive Goldstone mode is not discussed in the MI phase since the order parameter is zero in the thermodynamic limit. Likewise, no resonance is expected in the normal quantum critical liquid (NL), i.e., at finite temperature for critical parameters $(U, \mu) = (U_c, \mu_c)$. However, simulations reveal a resonance in the MI phase right after the gap threshold [1] suggesting that finite-energy probes are primarily sensitive to local correlations at length scales where MI and SF are indistinguishable. The universality of the MI response was likewise never clarified.

In this work, we aim to determine the universal scaling spectral functions when approaching the QCP not only from the SF, but also from the MI and NL phases. We rely on the worm algorithm [22, 23, 24] in the path integral representation to perform the required large-scale simulations. By collapsing spectral functions evaluated along the trajectories approaching to the QCP, we extract universal features for all three phases. They are summarized in Fig. 2.1, which is our main result. Surprisingly, all of them include a universal resonance peak (relatively sharp in SF and MI phases), followed by a broad secondary peak (in SF and MI phases).
phases only) before merging with the incoherent critical quasi-plateau (the plateau value is the same in all cases, as expected). Our results are in agreement with scaling theory, and firmly establish that the damped massive Goldstone mode(-like) survives in all three phases.

**Figure 2.1.** Universal spectral functions for scalar response in the superfluid, Mott insulator, and normal quantum critical liquid phases. For SF, the Higgs peak is at $\omega_H/\Delta = 3.3(8)$; for MI, $\omega_H/\Delta = 3.2(8)$; and for NL, $\omega_H/T = 6(1)$. There is a secondary peak around $\omega/\Delta \approx 15$ in the SF and MI phases, and all responses reach a quasi-plateau at the same height $0.6(1)$ at higher frequencies. The error bars on $\Phi_{SF,MI}$ come from the spread of collapsed curves, while the ones on $\Phi_{NL}$ are based on the variance of the analytical continuation results [1].

In the SF phase, to reliably extract the universal spectral function, we fine tune the system to the QCP more than an order of magnitude closer than the previous study [1]. The universal spectral function we finally calculated $\Phi_{SF}$ has three distinct features: a) A pronounced peak at $\omega_H/\Delta \approx 3.3$, which is associated with the massive Goldstone resonance. Since the peak’s width $\gamma/\Delta \approx 1$ is comparable to its energy, the Higgs mode is strongly damped. It behaves as a well-defined particle only in a moving reference frame; b) A minimum and another
broad maximum between $\omega/\Delta \in [5, 25]$ which may originate from multi-massive-Goldstone modes [1]; c) the onset of the quantum critical quasiplateau, in agreement with the scaling hypothesis (2.1), starting at $\omega/\Delta \approx 25$.

In the MI phase, the universal spectral function is found to be remarkably similar to its SF counterpart featuring a sharp resonance peak, and thus we interpreted it as a massive-Goldstone(-like) resonance. The standard picture of the massive Goldstone mode is in terms of amplitude oscillations of the order parameter in the Mexican hat potential. This picture is manifestly absent in the MI at distances exceeding the correlation length $\xi$. Therefore, this observation of the massive-Goldstone(-like) resonance is rather counter-intuitive. Our understanding is based on the picture that finite energy collective modes probe system correlations predominantly in a finite space-time volume. The resonance in the MI phase is an indication that for small $g$ and large correlation length $\xi \propto g^{-\nu}$ the effective action $F(\Psi)_R$ for the order parameter coarse-grained over length-scales $R \ll \xi$ still features a Mexican hat potential with strongly renormalized properties. This potential defined under the correlation length ultimately gives rise to the damped massive Goldstone resonance at frequencies exceeding the MI gap. We note that since the MI and SF are separated by a critical line their scaling functions $\Phi_{\text{MI}}$ and $\Phi_{\text{SF}}$ remain fundamentally different at energies smaller than $\omega_H$. We also point that the same argument can be applied to the NL phase in order to explain the similar resonance peak in the universal scaling function $\Phi_{\text{NL}}$, as shown in the Fig. 2.1.

### 2.2 The Method

We study the massive Goldstone mode with quantum Monte Carlo simulations of the homogeneous Bose-Hubbard model Eq. (1.1). The phase diagram of the 2D Bose-Hubbard model, shown in Fig. 2.2, is known with high accuracy [19, 2, 20] at both zero and finite temperature. The QCP is located at $U_c = 16.7424(1)$, $\mu_c = 6.21(2)$. When the system is
slightly detuned from the QCP, either by changing the chemical potential or the interaction strength, we define the corresponding characteristic energy scale $\Delta$ using the energy gap in the MI phase, $E_{\text{gap}}(g)$, by the rule illustrated in Fig. 2.2: For positive $g = (U - U_c)/J$ it is half the gap, $\Delta(g > 0) = E_{\text{gap}}(g)/2$, where $E_{\text{gap}} = \mu_c^+(\mu_c^-)$ is deduced from the upper and lower critical chemical potentials for a given $g$. For $g < 0$ along the trajectory i in the SF phase it is $\Delta(g < 0) = E_{\text{gap}}(-g)/2$. For $U = U_c$ and negative $g_\mu = (\mu - \mu_c)/J$ along the trajectory ii in the SF phase we first find $g$ such that $\mu_c^-(g) = \mu$ and then define $\Delta(g_\mu) = CE_{\text{gap}}(g)/2$ where the constant $C = 1.2$ (see below) is fixed by demanding that the universal function is the same along both SF trajectories. Note that $E_{\text{gap}}(g)$ in the thermodynamic limit can be determined accurately from the imaginary time Green function data [2] and finite-size scaling analysis.

To study the scalar response, we can imagine adding a small uniform modulation term to the Hamiltonian Eq.(1.1),

$$
\delta H(t) = -\delta J \cos(\omega t) \sum_{<ij>} b_i^\dagger b_j \equiv \frac{\delta J}{J} K(t),
$$

where $\delta J/J \ll 1$. The imaginary time correlation function for kinetic energy, $\chi(\tau) = \langle K(\tau)K(0) \rangle - \langle K \rangle^2$, is related to $S(\omega)$ through the spectral integral with the finite-temperature kernel, $N(\tau, \omega) = e^{-\omega \tau} + e^{-\omega(1/T-\tau)}$:

$$
\chi(\tau) = \int_0^{+\infty} N(\tau, \omega) S(\omega) d\omega.
$$

The spectral function $S(\omega)$ discussed in this chapter is sometimes called the dynamic structure factor in other literature. This function is related to the imaginary part of the retarded Green’s function $\chi(\omega) = \langle [\hat{K}(t), \hat{K}(0)] \rangle_\omega$ through the fluctuation-dissipation theorem, namely $S(\omega) = 2Im\chi(\omega)/(1 - e^{-\omega/T})$. At sufficiently low temperature, the additional factor becomes negligible.
Figure 2.2. (Color online) Ground state phase diagram of the Bose-Hubbard model in the vicinity of the QCP marked by a large (blue) dot (based on Ref. [2] data). The (blue) dashed curves specify trajectories in parameter space used to detune the system away from the QCP (trajectories i and iii correspond to unity filling factor $n = 1$, trajectory ii has constant interaction strength). The (black) lines with arrows explain how the characteristic energy scale $\Delta$ is obtained for these parameters (see text). The inset shows the phase diagram at finite temperature, and the trajectory taken in the NL phase.

We employ the same protocol of collecting and analyzing data as in Ref. [1]. More specifically, in the MC simulation we collect statistics for the correlation function at Matsubara frequencies $\omega_n = 2\pi T n$ with integer $n$

$$\chi(i\omega_n) = \langle K(\tau) K(0)\rangle_{i\omega_n} + \langle K \rangle$$

(2.4)

which is related to $\chi(\tau)$ by a Fourier transform. In the path integral representation, $\chi(i\omega_n)$ has a direct unbiased estimator, $|\sum_k e^{i\omega_n \tau_k}|^2$, where the sum runs over all hopping transitions in a given configuration, i.e. there is no need to add term (2.2) to the Hamiltonian explicitly.
Once $\chi(\tau)$ is recovered from $\chi(i\omega_n)$, the analytical continuation methods described in Ref. [1] are applied to extract the spectral function $S(\omega)$. A discussion on the reproducibility of the analytically continued results for this type of problem can also be found in Ref. [1].

We consider system sizes significantly larger than the correlation length by a factor of at least 4 to ensure that our results are effectively in the thermodynamic limit. Furthermore, for the SF and MI phases, we set the temperature $T = 1/\beta$ to be much smaller than the characteristic Higgs energy, so that no details in the relevant energy part of the spectral function are missed.

2.3 Numerical Results

We consider two paths in the SF phase to approach the QCP: by increasing the interaction $U \rightarrow U_c$ at unity filling factor $n = 1$ (trajectory i perpendicular to the phase boundary in Fig 2.2), and by increasing $\mu \rightarrow \mu_c$ while keeping $U = U_c$ constant (trajectory ii tangential to the phase boundary in Fig 2.2). We start with trajectory i by considering three parameter sets for $(|g|, L, \beta)$: $(0.2424, 20, 10)$, $(0.0924, 40, 20)$, and $(0.0462, 80, 40)$. The prime data in imaginary time domain are shown in Fig. 2.3 using scaled variables to demonstrate collapse of $\chi(\tau)$ curves at large times. Analytically continued results are shown in the inset of Fig. 2.4. After rescaling results according to Eq. (2.1), we observe data collapse shown in the main panel of Fig. 2.4. This defines the universal spectral function in the superfluid phase $\Phi_{SF}$.

When approaching the QCP along trajectory ii, with $(|g_\mu|, L, \beta) = (0.40, 25, 15)$, $(0.30, 30, 15)$, and $(0.20, 40, 20)$ we observe a similar data collapse and arrive at the same universal function $\Phi_{SF}$; see Fig. 2.5. The final match is possible only when the characteristic energy scale $\Delta(g_\mu) = C\Delta(g(g_\mu))$ involves a factor of $C = 1.2$.

The universal spectral function $\Phi_{SF}$ has three distinct features: a) A pronounced peak at $\omega_H/\Delta \approx 3.3$, which is associated with the Higgs resonance. Since the peak’s width $\gamma/\Delta \approx 1$ is comparable to its energy, the Higgs mode is strongly damped. It behaves as a well-defined
Figure 2.3. (Color online) Collapse of correlation functions in imaginary time domain for different values of $U$ along trajectory i in the SF phase, labeled by the detuning $g = (U - U_c)/J$.

particle only in a moving reference frame; b) A minimum and another broad maximum between $\omega/\Delta \in [5, 25]$ which may originate from multi-Higgs excitations [1]; c) the onset of the quantum critical quasiplateau, in agreement with the scaling hypothesis (2.1), starting at $\omega/\Delta \approx 25$. These features are captured by an approximate analytic expression with normalized $\chi^2 \sim 1$,

$$\Phi_{SF}(x) = \frac{0.65x^3}{35 + x^{2/\nu}} \left[ 1 + \frac{7 \sin(0.55x)}{1 + 0.02x^3} \right]$$

We only claim that a plateau is consistent with our imaginary time data and emerges from the analytic continuation procedure which seeks smooth spectral functions; i.e., other analytic continuation methods may produce an oscillating behavior in the same frequency range within the error bar in Fig. 2.1.

In the MI phase we approach the QCP along trajectory iii in Fig 2.2. The scaling hypothesis for the spectral function has a similar structure to the one in Eq. (2.1),
Figure 2.4. (Color online) Collapse of spectral functions for different values of $U$ along trajectory i in the SF phase, labeled by the detuning $g = (U - U_c)/J$. Inset: Original data for $S_{SF}(\omega)$.

$$S_{MI}(\omega) \propto \Delta^{3-2/\nu} \Phi_{MI}(\frac{\omega}{\Delta}).$$  \hfill (2.6)

The low-energy behavior of $\Phi_{MI}$ starts with the threshold singularity at the particle-hole gap value, $\Phi_{MI}(x) \approx 1/\log^2(4/(x-2))\theta(x-2)$, see Ref. [34]. At high frequencies $\Phi_{MI}(x \gg 1)$ has to approach the universal quantum critical quasiplateau (same as in the SF phase). Our results for the spectral functions at $g = 0.2576$ (with $L = 20, \beta = 10$) and $g = 0.1276$ (with $L = 40, \beta = 20$) are presented in Fig.2.6. The universal scaling spectral function shows an energy gap (this is also fully pronounced in the imaginary time data). The left-hand side of the first peak is much steeper than in the SF phase, in agreement with the theoretical prediction for the threshold singularity.

The universal spectral function in the MI is remarkably similar to its SF counterpart featuring a sharp resonance peak. (Since MI and SF are separated by a critical line their
scaling functions $\Phi_{\text{MI}}$ and $\Phi_{\text{SF}}$ remain fundamentally different at energies smaller than $\omega_H$).

This observation is rather counterintuitive given that the superfluid order parameter is zero and raises a number of theoretical questions regarding the nature and properties of collective excitations in the MI phase at finite energies. In particular, can it be linked to the established picture of renormalized free-energy functional for the order parameter field [36] at distances under the correlation length?

If finite energy excitations probe system correlations predominantly in a finite space-time volume, one would expect that some resonant feature may survive even in the NL phase at sufficiently low, but finite temperature $T < J$ (at $g = g_\mu = 0$, the superfluid transition temperature is zero) In this quantum critical region, temperature determines the characteristic energy scale, thus $S_{\text{NL}}(\omega) \propto T^{3-2/\nu}\Phi_{\text{NL}}(\omega/T)$, and all excitations are strongly damped. Simulations performed at $T/J = 0.5$ on the trajectory iv in the inset of Fig. 2.2 indeed find a peak at low energies before the critical quasiplateau, see Fig. 2.1, but it is much less
Figure 2.6. (Color online) Collapse of the spectral functions for different $U$ along trajectory iii in the MI phase, labeled by the detuning $g = (U - U_c)/J$. Inset: Original data for $S_{\text{MI}}(\omega)$.

pronounced and the oscillatory component (second peak) is lost. Unfortunately, numerical complexity does not allow us to verify the scaling law directly by collapsing simulations at lower temperatures and bigger system sizes. Our case for universality of $\Phi_{\text{NL}}(x)$ is thus much weaker and rests solely on the theoretical consideration that the plateau (at the same value as in the SF and MI phases) separates universal physics from model specific behavior.

2.4 Conclusions

In conclusion, we have constructed the universal spectral functions $\Phi$ for the kinetic energy correlation function for all three phases in the vicinity of the interaction driven QCP of the 2D Bose-Hubbard model. Although the nature of excitations in these phases is fundamentally different at low temperature, their $\Phi$ functions all feature a resonance peak which in the SF and MI phases is followed by a broad second peak and evolve then to a quasiplatform at higher energy in agreement with scaling predictions. In the SF phase, the
first peak is interpreted as a damped Higgs mode. In the MI and NL phase, the existence of a resonance is unexpected and requires further theoretical understanding of amplitude oscillations at mesoscopic length scales. Experimental verification with cold gases requires flatter traps and lower temperatures and is accessible within current technology. It would signify a new hallmark, going beyond the previous studies of criticality near Gaussian fixed points.
CHAPTER 3
OBSERVING THE MASSIVE GOLDSTONE MODE IN ULTRACOLD ATOMS IN OPTICAL LATTICES

The text of this chapter has been adapted from Ref. [8].

3.1 Introduction

As discussed in the previous chapter, the fate of the MG-mode in 2D is an intriguing and controversial issue because its decay into lower-energy gapless modes is found to be strong. The mode was argued to become either completely overdamped (i.e., without any resonance type feature in spectral functions [27, 28, 29]) or be detectable as a well-defined resonance peak in certain spectral functions on the superfluid side away from (but not on approach to) the critical point [31, 32, 30].

Recent progress on ultracold atom in optical lattice experiment [3], as well as Monte Carlo simulations [1, 37, 7, 38], $1/N$ corrections to higher order [34], and non-perturbative renormalization group methods [39, 40] have presented solid evidence in favor of yet another scenario: A critical resonance in the universal scaling regime. Unlike MG-modes in three (and higher) dimensions which become sharper when approaching the QCP, the ratio of the width of the resonance peak over its mass remains constant in (2+1) dimensions.
In order to detect the MG-mode experimentally, the scalar spectral density $A(\omega)$ \(^1\) (i.e., the imaginary part of the retarded Green’s function of $|\Psi^2|$) is considered to be the best probe \([30]\). On the SF side of the transition point, in the scaling limit, $A(\omega)$ takes the form \([25]\)

$$A_{\text{SF}}(\omega) \propto \Delta^{3-2/\nu} \Phi_{\text{SF}}(\frac{\omega}{\Delta}),$$

(3.1)

where $\Delta$ is the Mott insulator gap for the same amount of detuning from the QCP, and $\nu = 0.6717$ is the correlation length exponent for the $U(1) \equiv O(2)$ universality in $(2 + 1)$ dimensions \([4, 35]\). The universal function $\Phi_{\text{SF}}(x)$ starts as $\Phi_{\text{SF}}(x \to 0) \propto x^3$ and saturates to a quasi-plateau with weak $\omega$ dependence $\Phi_{\text{SF}}(x \gg 1) \propto x^{3-2/\nu} \approx x^{0.0225}$. The intermediate regime between the two limits can be constructed numerically, where a well-defined resonance peak associated with the critical MG-mode is observed at $x = 3.3(8)$\([7]\). Monte Carlo data also suggest that a similar universal resonance, though less pronounced, may equally well be seen on the other side of the transition, as well as in the quantum critical normal liquid \([7, 38, 39]\). These conclusions are yet to be confirmed or refuted experimentally.

The bottleneck of the numerical analysis is analytical continuation of data for correlation functions from imaginary to real frequencies, $A(i\omega_n) \to A(\omega)$, where $i\omega_n = 2\pi nT$ with $n = 0, \pm 1, \pm 2 \ldots$ are Matsubara frequencies. This procedure is a notorious, ill-posed problem that requires application of certain regularization schemes \([41, 5]\), and thus independent experimental studies are required for final understanding.

The ultracold atom experiment of Ref. \([3]\) aimed at detecting the MG-mode in $A_{\text{SF}}(\omega)$ and confirmed the expected softening of the quantum critical spectrum implied by (3.1) but remained inconclusive with regards to the existence of a well-defined MG resonance. To

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\(^1\)In this chapter, to closely connect with the ultracold atoms experiment where the temperature is finite, we study the spectral density $A(\omega)$ instead of the spectral function $S(\omega)$ used in the last chapter. Two quantities are related by the fluctuation-dissipation theorem $A(\omega) = (1 - e^{-\omega/T})S(\omega)$. The temperature-dependent factor becomes non-negligible at the experimental temperature.
obtain $A(\omega)$, a 2D Bose Hubbard system was gently ”shaken” by modulating the lattice laser intensity (lattice depth) and probed by in situ single-site- and single-atom-resolved measurements. The observed signal (through temperature increase) featured a broad maximum whose onset softened on approach to QCP, in line with the scaling law (3.1). The onset correlates remarkably well with the energy of the MG-mode, while the ratio of the onset width to its frequency was measured to be approximately constant when approaching the critical point. However, a resonance-type peak with diminishing width was not detected, which can be interpreted either as evidence for the MG-mode being overdamped in the critical state or as broadening caused by finite temperature and system inhomogeneity (tight confinement) effects [1]. Thus a direct comparison between numerical calculations and experimental measurements with a common setup is crucial to settle the controversy.

In this chapter, we employ an ab initio numerical procedure based on quantum Monte Carlo simulations and numerical analytic continuation [5] to calculate spectral density for ultra-cold atoms in optical lattices. The final result for the temperature increase as a function of modulation frequency successfully reproduces the main data of Ref. [3] for the experimental setup “as is”; i.e, in the spirit of the quantum simulation paradigm [33]. The consistency between numerical results and experimental measurements establishes the reliability of both approaches, and, in particular, validates the analytic continuation procedure. Moreover, simulations performed for various system parameters indicate several improvements/requirements with regards to the experimental setup that will help revealing the resonance peak in the spectral density. They include (i) the system should be effectively homogeneous to avoid inhomogeneous broadening, which can be achieved through confining the lattice depth modulation locally at the parabolic trap center; (ii) the detuning from the QCP should be small, $j/j_c \leq 1.05$, where $j = J/U$ is the dimensionless coupling parameter for the Bose Hubbard model introduced below [see Eq.(1.1)], and $j_c$ is its critical value; and (iii) the system’s temperature should be at least as low as the Berezinskii-Kosterlitz-Thouless
transition point $T_c$. Our results suggest that a direct observation of a well-defined resonance peak and understanding the fate of the MG-mode experimentally is challenging but not impossible.

The rest of the paper is organized as follows. We introduce the model in Sec. 3.2 and describe the numerical procedure in Sec. 3.3. The comparison between the temperature response from simulations and experimental measurements in a specific setup from Ref. [3] is presented in Sec. 3.4. We discuss requirements and possible experimental improvements to reveal the MG resonance in Sec. 3.5.

3.2 The model

Ultracold bosons in optical lattices offer unique possibilities to study the SF-MI quantum phase transition in 2D [15, 16]. At low enough temperatures the physics of the system is restricted to the lowest Bloch band, and can be described by the Bose-Hubbard (BH) model [17, 18], which is parametrized by a hopping amplitude $J$ and an on-site interaction energy $U$,

$$
\hat{H}_0 = -J \sum_{\langle i,j \rangle} (b_i^\dagger b_j + H.c.) + \frac{U}{2} \sum_i n_i(n_i - 1) - \sum_i (\mu - V_i)n_i,
$$

where $b_i^\dagger \ (b_i)$ creates (annihilates) a particle on the site $i$, and $\langle i, j \rangle$ denotes the sum over nearest neighbors on the square lattice. In the BH model, the dimensionless coupling parameter $j = J/U$ is easily tunable via the lattice depth, and the dimensionality of the system can be reduced to 2D by suppressing the hopping in the third direction. The total particle number $N$ is controlled by the global chemical potential $\mu$. Finally, an ultracold atomic gas is trapped by a confining potential $V_i$, which is usually harmonic, $V_i = \frac{1}{2} m \omega^2 d^2 R_i^2$ (with $m$ the mass of atom, $d$ the lattice spacing, and $R_i$ the distance of site $i$ from the trap center measured in units of $d$). Within the local density approximation picture (LDA), $\mu - V_i$ plays the role of a local chemical potential.
Ideally, without the $V_i$ term in Eq. (3.2), the system is a homogeneous 2D Bose Hubbard model and its phase diagram is known with high accuracy [19, 2, 20] at both zero and finite temperature. In the ground state, the system undergoes a second order phase transition from the SF to the MI when decreasing the ratio $j = J/U$ at fixed integer filling factor. At filling factor $\langle n \rangle = 1$, the transition occurs at $j_c^{-1} = 16.7424(1)$ and $\mu_c/J = 6.21(2)$ and features a QCP with emergent particle-hole symmetry, which enlarges the Galilean invariance to Lorentz invariance (the system is actually conformally invariant). The SF phase is supposed to have the critical MG-mode according to the discussion in the previous section.

When the $V_i$ term is presented as in current experimental implementations [3], due to the inhomogeneous local chemical potential, the particle density decreases to zero when moving away from the center of the trap. Any conclusion regarding the existence of the GM-resonance in the homogeneous case cannot be naively applied to the realistic experiment, even if the center of the atomic system is fine-tuned to be in the vicinity of QCP. A careful bottom-up calculation of the scalar spectral density is required in order to understand the experimental signal.

### 3.3 Spectral density measurement: Theory

In this section, we revisit the generic mathematical framework for the measurement of the scalar spectral density in ultracold atoms.

In the BH model, the total kinetic energy $\hat{K} = -J \sum_{\langle i,j \rangle} (b_i^\dagger b_j + H.c.)$ is the simplest operator with nontrivial dynamics leading to strong scalar response. Thus, we may consider adding an external perturbation term $\delta f(t) \hat{K}$ to the Hamiltonian (3.2). Within standard linear response theory, the total kinetic energy response is proportional to the external field, and the ratio defines the response function $\chi(\omega, T) \equiv \delta \langle \hat{K}(\omega) \rangle_T / \delta f(\omega)$ where $\langle ... \rangle_T$ denotes the thermal average at temperature $T$. The spectral density is defined as the dissipative
part of the response function, \( A(\omega, T) \equiv 2\text{Im}\chi(\omega, T) \), so that \( A(\omega, T) \) is proportional to the energy absorbed by the system, which, in turn, determines the temperature change of the system. To learn about the spectral density, one can measure either the total kinetic energy response or the temperature change. Though being rather indirect, the latter one is the quantity that is measurable in the ultracold atom experiment [3].

Experimentally, a small uniform modulation \( \delta V_0 \cos(\omega t) \) of the optical lattice depth \( V_0 \) is applied in the 2D plane to generate the external perturbation term [42, 3]. In the parameter regime where the BH model is a valid approximation, the lattice depth in units of the recoil energy \( E_r = \frac{\pi^2}{2md^2} \) is much larger than unity and controls both parameters \( J \) and \( U \): \( J \approx \frac{4}{\sqrt{\pi}} E_r (V_0/E_r)^{3/4} e^{-2\sqrt{V_0/E_r}}, U \propto (V_0/E_r)^{D/4} \) [16] where the effective dimension \( D = 2 \). Substituting \( V_0 \) with \( V_0 + \delta V_0 \cos(\omega t) \) in \( J \) and \( U \), and keeping terms to first order in \( \delta V_0 \), the perturbed BH Hamiltonian reads

\[
\hat{H}(t) = \hat{H}_0 + \delta g(t)\hat{H}_0 + \delta g(t) \sum_i V_i \hat{n}_i + \delta f(t)\hat{K} \tag{3.3}
\]

Here, the generalized forces \( \delta f(t) = \delta f_0 \cos(\omega t) \) with \( \delta f_0 = \frac{1}{4} - \sqrt{V_0/E_r} \frac{\delta V_0}{\delta V_0} \) and \( \delta g(t) = \delta g_0 \cos(\omega t) \) with \( \delta g_0 = \frac{\delta V_0}{2 \sqrt{V_0}} \) are linear in \( \delta V_0 \). Note that the second term in Eq.(3.3) commutes with \( H_0 \) and yields no contribution to the spectral density. Furthermore, we argue that the effect from the confining potential term (third term) is also negligible compared to the kinetic energy term (fourth term) if one of the following conditions is satisfied: (i) \( |\delta g_0/\delta f_0| = 2/(4\sqrt{V_0/E_r} - 1) | \ll 1 \); and (ii) the trap is large enough and LDA is valid; namely, it is possible to decompose the system into independent mesoscopic regions whose sizes are larger than the correlation length but are still small enough to be regarded as homogeneous systems with the local chemical potential \( \mu - V_i \). This implies, on the one hand, that the total response of the system can be approximated by a sum over independent contributions from mesoscopic regions, while, on the other hand, the confining potential
term in each mesoscopic region is proportional to the particle number in this region and thus
commutes with the local $H_0$ (i.e., it is not dynamic under LDA). The combined effect is that
the confining potential does not contribute to the linear response. The validity of LDA for
critical systems has been addressed before in Ref. [43].

For ultracold atoms whose dynamics is dominated by the kinetic energy term, the energy
dissipation rate is proportional to the kinetic energy spectral density $A(\omega)$,

$$\dot{E}(\omega, T) = \frac{\omega}{4} A(\omega, T) \delta f_0^2 + P(\omega, T). \quad (3.4)$$

Here $P(\omega, T)$ is the heating power from other mechanisms (ultracold atoms are always cou-
pled to the photon subsystem and are subject to collisions with the background gas). In the
leading approximation, $P$ does not depend on the small lattice-depth modulation, and we
expect $P(\omega, T) \approx P(T)$.

Assuming that the system is quasistatic, i.e., the relaxation time is small enough, $\tau \ll 1/\omega$, the thermodynamics can applied at all times and the final temperature shift can be
deduced from the following self-consistent equation,

$$T(\omega, t) - T(\omega, 0) = \int_0^t \frac{\dot{E}(\omega, T(\omega, t'))}{C(T(\omega, t'))} \, dt' \quad (3.5)$$

where $t$ is the period of the modulation and $C(T)$ is the heat capacity. We do not assume
here that under the linear response conditions one is allowed to neglect the time dependence
of temperature on the right hand side (r.h.s.) of Eq. (3.5). This is because over long
modulation times the temperature change might be substantial. In the experiment [3], the
initial temperature is chosen to be frequency independent, $T(\omega, 0) = T_{\text{ini}}$, and the modulation
time to be a certain fixed number of modulation cycles $t = t(\omega) = 2\pi M/\omega$. Then the final
temperature dependence on frequency, $T_{\text{fin}}(\omega) = T(\omega, t(\omega))$, is directly related to $A(\omega)$, and
any sharp resonance structure in $T_{\text{fin}}(\omega)$ can be traced back to the spectral density, i.e., the temperature response provides a practical probe to detect the MG-mode as demonstrated in Ref. [3].

### 3.4 Measuring the spectral density in simulations

In this section, the experimental setup from Ref. [3] is used as a benchmark system for calculation of the temperature response from first principles. The parameters closest to the QCP include the lattice depth $V_0 = 10E_r$, which gives a dimensionless coupling parameter $j/j_c = 1.2$ (or $U = 14J$), and the particle number $\langle N \rangle = 190(36)$. Combined with the unity filling requirement at the trap center, this corresponds to the harmonic confinement $V_i/J = 0.0915(x_i^2 + y_i^2)$. [1] The small dimensionless modulation of the lattice depth is $\delta V_0/V_0 \approx 0.03$, which corresponds to the generalized forces $|\delta f_0| = 0.087$ and $|\delta g_0| = 0.015$. Those parameters define the perturbed BH model (3.3).

We argue that the external potential term in Eq. (3.3) is negligible, since both conditions discussed in the previous section are fulfilled: (i) $|\delta g_0/\delta f_0| = 0.17 \ll 1$ and (ii) the correlation length near the trap center at a typical experimental temperature is about one lattice spacing [1], so that the LDA also holds in the vicinity of the trap center, which dominates the total response.

In the experiment, the modulation protocol consists of two stages. First, ultracold atoms are modulated for $M = 20$ oscillation cycles. Second, the system is held to thermalize for some time such that the sum of modulation and hold time is constant at 200 milliseconds for all modulation frequencies. During the first stage, both the modulation and the heating power $P(T)$ contribute to the system’s energy dissipation, while during the second stage, only the heating power $P(T)$ contributes to the energy increase. The integral over time in Eq. (3.5) must hence be divided into two segments in order to correctly account for both modulation and holding stages. The advantage of keeping the two-stage time at the same
value is that the contribution of $P(T)$ is essentially constant for all modulation frequencies. Finally, the temperature $T_{\text{fin}}(\omega)$ is determined by slowly ramping the system to the atomic limit and measuring the atomic parity in situ with single-site resolution.

We rely on path-integral quantum Monte Carlo (MC) simulations with worm-type updates [23, 24] to calculate the scalar spectral densities and the specific heat. Since the particle loss in the experiment is negligible, we simulate the system in the canonical ensemble.

In MC simulations, it is straightforward to measure the imaginary time correlation function for the kinetic energy, 

$$
\chi(\tau) = \langle K(\tau)K(0) \rangle_T - \langle K \rangle_T^2,
$$

which is related to $A(\omega)$ via the spectral integral

$$
\chi(\tau) = \int_0^{+\infty} \frac{d\omega}{2\pi} N(\tau, \omega; T) A(\omega),
$$

(3.6)

with the finite-temperature kernel, 

$$
N(\tau, \omega; T) = 2(e^{-\omega\tau} + e^{-\omega(1/k_B T - \tau)})/(1 - e^{-\omega/k_B T}).
$$

We employ the same protocol for collecting and analyzing data as in Refs. [1, 7]. More precisely, we collect statistics for the correlation function at Matsubara frequencies $\omega_n$

$$
\chi(i\omega_n) = \frac{1}{\beta} \langle |K(i\omega_n)|^2 \rangle_T + \langle K \rangle_T,
$$

(3.7)

and recover $\chi(\tau)$ by a Fourier transform. In the path-integral representation, $\chi(i\omega_n)$ has a direct unbiased estimator, $|\sum_k e^{i\omega_n \tau_k}|^2$, where the sum runs over all hopping transitions in a given configuration. Once $\chi(\tau)$ is obtained from $\chi(i\omega_n)$ with an accuracy up to $10^{-4}$ the analytic continuation method described in Ref. [5] is applied to extract the spectral density $A(\omega)$. We present the analytically continued results at different temperatures in Fig.3.1, where we see that the curves look qualitatively similar at all temperatures in the range between $0.5J/k_B$ and $3.33J/k_B$; values of $A(\omega; T)$ at any temperature in this range can be estimated using linear interpolation. All spectral densities vanishing at zero frequency reflects the absence of dissipation in response to a static external field. Another way to understand this result is through the dissipation-fluctuation theorem,

$$
A(\omega; T) = (1 - e^{-\omega/k_B T}) S(\omega; T)
$$
where $S(\omega; T)$ is the dynamic correlation function of kinetic energy. Zero value of $A(\omega = 0; T)$ is a natural outcome of a finite $S(\omega = 0; T)$, see Fig. 6 in Ref. [1]. We also would like to point out that the analytical continuation result becomes unreliable at very low frequency $\omega \ll 1/\beta$ when the spectral weight is relatively small.

![Figure 3.1](image)

**Figure 3.1.** Spectral densities of the kinetic energy per atom at different temperatures for the experimental setup of Ref. [3]. All curves look qualitatively similar.

The heat capacity for a canonical-ensemble system has also been calculated and is shown in Fig. 3.2. It is seen that the heat capacity becomes much smaller in the superfluid phase than in the normal phase, which may lead to more rapid heating.

To solve Eq. (3.5) self-consistently, the initial temperature $T_{ini}$ and the heating power $P(T)$ are also required. However, both quantities were not addressed by the previous experiment nor is $P(T)$ computable by Monte Carlo simulations. Thus, we are forced to consider both quantities as fitting parameters. In Fig. 3.3, we show two possible temperature responses to modulation obtained by solving Eq. (3.5), which both fit the experimental data well despite having rather different (but realistic) sets of $(T_{ini}, P)$. Excellent agreement between
the numerical and experimental results not only ensures that the analytical continuation procedure (as routinely applied on the kinetic energy correlation function [1, 7, 37, 38, 39]) is reliable, but also validates various assumptions made in the first-principle calculation, such as quasi-static thermodynamics. We also would like to point out that there are no fundamental difficulties in experiment to measure $T_{\text{ini}}$ and $P(T)$, and thus an even more stringent test avoiding any fitting can be envisioned in the future.

![Heat capacity plot](image)

**Figure 3.2.** Heat capacity $C(T/J)$ per atom as a function of temperature $T/J$. For the homogeneous system, the Berezinskii-Kosterlitz-Thouless transition temperature is at $k_B T_c \approx 1.04J$. [2] Notice that below $T_c$, the heating of the system gets boosted due to the smallness of $C(T/J)$.

### 3.5 On the experimental observation of the massive Goldstone peak

Comparing the temperature response in Fig. 3.3 with the spectral density for a homogeneous system with $j/j_c = 1.2$ (or $U = 14J$) (see Fig. 2 of Ref. [1]), we find that while the
steep onset of the spectral weight correlates remarkably well with the GM-mode energy, the resonance structure is lost in the experimental system. As mentioned previously, this may occur for two unrelated reasons: either because the MG-mode is overdamped, or the resonant signal is broadened by finite temperature and system inhomogeneity (tight confinement) effects [1].

Our simulations indicate that the second scenario is far more likely. Previous work on the homogeneous case established that a detuning smaller than \( j/j_c = 1.05 \) (or \( U = 16 \)) is required to clearly see the MG-resonance on top of the high-frequency continuum. Let us therefore take a system with \( j/j_c = 1.05 \), particle number \( N = 800 \) and unity filling factor at the trap center and perform a numerical thought experiment: in order to reduce
inhomogeneity effects, we limit the lattice-depth modulation to a mesoscopic area around the trap center, where the confining potential is nearly flat. For simplicity, we choose a square area with side length $R$. In Fig. 3.4, we show spectral densities for different values $R$. Resolving the resonance structure hiding in the inhomogeneous signal is dramatically improved when the modulation area is reduced. Though no resonance structure is seen when the entire system is modulated ($R/d = \infty$), it emerges when the modulation region is reduced to $R/d = 16$ or $R/d = 8$ at low enough temperature $T \sim T_c$ (where $T_c \approx 0.45J/k_B$ is the BKT temperature for a homogeneous model with $j/j_c = 1.05$). Converting spectral density to temperature response does not change this observation qualitatively, see Fig. 3.4, even though the contrast for observing the resonance feature is diminishing. This thought experiment demonstrates that by taking care of response homogeneity, detuning from the QCP, and temperature, the MG-peak can be seen in the kinetic energy spectral density using existing technology.

Combining the numerical results for the homogeneous and inhomogeneous model from Refs. [1, 7] and from this work, we deduce that the following three conditions are to be met in order to reveal the MG-peak:

First, the modulation area should be restricted to the region with nearly constant chemical potential to ensure that the temperature response is measured for a homogeneous system. To achieve it, a straightforward approach would be to replace the harmonic confinement with the flat-bottom plus sharp walls potential. This approach, however, may lead to problems with controlling system’s density and entropy, and, thus, detuning from the QCP. An alternative approach is to restrict modulation to a mesoscopic area around the trap center, as shown is done in Fig. 3.5. One promising experimental implementation would be to apply a localized modulation of the scattering length [44] using a laser beam induced Feshbach resonance [45]. The technique has recently been shown in ultracold atom without optical lattice [46, 47]. The size of the modulation area can be engineered by tuning the size of
the laser beam (e.g. using a mask). Such a modulation would result in a time-dependent on-site interaction $U$ in the modulation area. As pointed out in Sec. 3.3, by subtracting a term proportional to $H_0$, the perturbation in potential energy can be replaced with the perturbation in kinetic energy, meaning that the MG-mode can be studied using the same temperature-response protocol as in the current experiment.

Second, the system has to be close enough to the QCP so that a Lorentz invariant action provides an adequate description of physics. Our simulations indicate that a detuning $j/j_c \lesssim 1.05$ is sufficient to reveal the MG-resonance, while a smaller detuning $j/j_c \lesssim 1.02$ is required to recover the universal spectral density Eq. (3.1) including the critical pseudo-plateau at large frequencies [7].

Third, the system temperature has to be low enough. For a homogeneous system, simulations suggest that the resonance peak survives at temperatures as high as the BKT transition temperature $T_c$, but gradually goes away at $T > 2T_c$ [1]. Thus, having initial temperatures below $T_c$ is recommended. For example, in the test system with $j/j_c = 1.05$, $N = 800$, and localized modulation size $R = 8d$, which heats from $T_c$ up to $2T_c$ ($T_c \simeq 0.45J/k_B$), the resonance peak will remain visible in temperature response according to Fig. 3.4(c).

### 3.6 Conclusions

To conclude, we would like to point out that the quantum critical dynamics in the MI and normal liquid phases is also of great interest. Numerical simulations indicate the presence of a universal resonance structure in the spectral density not only in the SF phase but also in phases with un-broken $U(1)$ symmetry, and at temperatures $T \gg T_c$ (normal quantum critical liquid) [7]. The existence of such universal resonances is unexpected within the current weak-coupling theory and their nature requires further study. Verification of this prediction from ultracold atom experiments would be crucial to solve this puzzle.
Figure 3.4. Spectral densities for different modulation areas (a square of size $R \times R$ whose center coincides with the trap center) and temperatures for a system with $N = 800$ atoms and $j / j_c = 1.05$. The MG-resonance emerges at temperatures $T \sim J / k_B$ when the modulation is limited to a mesoscopic area of linear size $R = 16d$, where $d$ is the lattice spacing.
Figure 3.5. Temperature response for different modulation areas for the same sets of model parameters as in Fig 3.4. We assume the system’s heating power to be $P = 0.2\,\text{J/sec}$ and the initial temperature $k_B T/J = 0.5$. To optimize the contrast, the number of modulation cycles is set to be three and the sum of modulation and hold time is kept constant at 19 milliseconds. The best modulation strength are found to be $\delta V_0/V_0 = 0.02, 0.03, 0.06$ for $R/d = 8, 16, \infty$ respectively.
4.1 Introduction

Transport properties of systems in the quantum critical region near zero-temperature have been a subject of intense theoretical and experimental studies for decades. Systems in two spatial dimensions fall in a particularly challenging class: Due to strong fluctuations standard mean field and perturbative methods fail, rendering the problem notoriously difficult and controversial. The optical conductivity, \( \sigma(\omega) \), is the key transport property describing the response of particles to an externally applied frequency dependent chemical potential gradient, or “electric” field [25]. QCP in two-dimensional models with \( O(2) \) symmetry have emergent symmetry larger than Lorentz symmetry, conformal invariance, described by a conformal field theory (CFT). The conductivity then has zero scaling dimension and follows the scaling law [48],

\[
\sigma(\omega, T \to 0) = \sigma_Q \Sigma(\omega/T), \quad \text{with} \quad \sigma(\omega/T \to \infty) \to \sigma(\infty),
\]

where we set \( \hbar = k_B = 1 \) as units. The conductivity quantum, \( \sigma_Q = 2\pi Q^2 \) (see Ref. [49]), absorbs the coupling constant to the external field used to induce the gradient in the chemical potential, \( e.g. \), the electric charge \( Q \) leaving \( \Sigma(x) \) a dimensionless, universal scaling function.
Theoretically, a perturbative approach based on the leading order term in both the $\epsilon = 3 - d$ and $1/N$ expansions has limited power to predict the quantitative and even qualitative properties of $\Sigma(x)$ in $d = 2$ and $N = 2$[25, 49, 48, 50]. This impasse was broken by the promising introduction of the AdS/CFT or holographic correspondence from string theory to condensed matter physics[51, 52, 53]. The main results of the correspondence of interest to this work are that the strongly coupled CFT in the quantum critical region can be mapped onto a weakly coupled gravity theory in Anti de Sitter space (AdS), where $\Sigma(x)$ can be computed by standard perturbative techniques[11, 54]. When holographic theory is approximated by a classical gravity theory (and truncated to terms up to four derivatives) the final result for $\Sigma(x)$ has only two free parameters: $\Sigma(\infty)$ and $\Sigma(0)$, or $\gamma = (\Sigma(0) - \Sigma(\infty))/4\Sigma(\infty)$, meaning that the shape of the universal $\Sigma(x) - \Sigma(\infty)$ curve is completely determined by $\gamma$.

The charge transport could either be particle-like for $\gamma > 0$ or vortex-like for $\gamma < 0$, where causality further constrains the value of $\gamma$ to be $|\gamma| \leq 1/12$[11, 52].

In this work, we establish an accurate estimate of the $\sigma(\infty)$ parameter which is (i) the key dynamic characteristic of the quantum critical continuum, and (ii) the most robust property of the quantum critical point, e.g. it is stable against disorder. We found that it was necessary to simulate system sizes that are at least an order of magnitude larger than in previous studies, which in turn required that the location of the QCP be refined to six significant digits. Only then were we able to deduce the universal function $\sigma(i\omega_n) - \sigma(\infty)$ with error bars suitable for precise tests of analytic theories, in particular the holographic theory[11]. We find that the holographic correspondence with temperature of the black brane horizon, $T_B$, equal to $T$ [11, 54] cannot account for the data. The fit works better if one includes $T_B$ to the set of fitting parameters suggesting that the theory can be renormalized [54]. To go from the Matsubara to the real-frequency axis we fit the data by using a simple analytical form and obtain results consistent with the particle-like transport (as opposed to vortex-like transport). By simulating the quantum critical liquid state of the Bose-Hubbard
model, we shed light on the possibility of measuring the universal conductivity with ultracold atoms in optical lattices.

We also point out that the recent development of the holographic theory has found a new relevant term in the quantum gravity action. The modified theory is claimed to be compatible to our data without any rescaling on the temperature of the black hole[12].

4.2 Models

Our simulations were performed for the three-dimensional classical J-current model [21] with $L^2 \times L\tau$ sites,

$$H = \frac{1}{2K} \sum_{<ij>} \nabla J = 0 \sum_{<ij>} J^2_{<ij>},$$

(4.2)

where $J_{<ij>} \in (-\infty, \infty)$ are integer valued bond currents between the neighboring sites subject to the zero-divergence constraint such that the allowed configurations form closed loops. The same approach was used in Refs. [55, 56]. In Fig. 4.1 we show our data for the winding numbers squared for different system sizes. The crossing point determines the location of the critical parameter in the J-current model. Our result $K_c = 0.3330670(2)$ is consistent with previous estimates [57, 58] but is far more accurate. As explained in the next section, if $K_c = 0.33305$ is used instead, the data are dramatically affected by that.

We also simulated the 2d quantum Bose-Hubbard mode Eq. (1.1) at the superfluid–Mott-insulator quantum critical point.

4.3 Methods

For both classical and quantum models, the conductivity in Matsubara representation is given by [59, 60, 49],

$$\sigma(i\omega_n) = 2\pi\sigma_Q \frac{\langle -k_x \rangle - \Lambda_{xx}(i\omega_n)}{\omega_n},$$

(4.3)
which is a direct consequence of the well-known Kubo formula. Matsubara frequencies are defined as $\omega_n = 2\pi n/\beta$ and $\omega_n = 2\pi n/L_\tau$ for the bosonic and classical systems, respectively. $\langle k_x \rangle$ is the kinetic energy associated with a $x$-oriented bond, $\Lambda_{xx}(i\omega_n)$ is the fourier transform of imaginary time current-current correlation function [59, 60]. The numerator has an unbiased estimator in the path integral representation of the Bose-Hubbard model, $1/\beta L^2 \langle |\sum_k \text{sgn}(k)e^{i\omega_n \tau_k}|^2 \rangle$, where the sum runs over all hopping transitions in a given configuration and $\text{sgn}(k)$ takes values $+1$ or $-1$ depending on the positive or negative direction of the $k$-th transition. A similar estimator can be applied to the J-current model. The conductivity on the real frequency axis, $\sigma(\omega)$, requires an ill-conditioned analytical continuation $i\omega_n \rightarrow \omega + i0^+$. To obtain the universal conductivity in the quantum critical region, one has to carefully extrapolate data to the infinite system size and zero temperature limits such that $L \rightarrow \infty$ is
taken first, and $L_{\tau} \to \infty$. The largest system size used in this study was $L = 1024, L_{\tau} = 512$ for the J-current model and $L = 400, \beta = 20/t$ for the Bose-Hubbard model. In the following subsections, we describe the details of two protocols used to eliminate finite-size and finite-temperature effects: the first one is used to obtain data for conductivity $\sigma(i\omega_n)$ in the Matsubara frequency representation in the thermodynamic limit $L \to \infty$ at fixed $L_{\tau}$ (in the classical case) or fixed $T$ (in the quantum case), and the second one is used to extrapolate the thus obtained thermodynamic limit data to the universal $L_{\tau} \to \infty$ (zero temperature) limit.

4.3.1 Finite system size extrapolation

![Figure 4.2. Extrapolating conductivity obtained for the first non-zero Matsubara frequency $\omega_1$ to the thermodynamic limit $L/L_{\tau} \to \infty$ for a fixed system size $L_{\tau} = 96$ in the $\tau$ direction (imaginary time). Unmodified [zero-winding sector] data are plotted with red circles [black squares]. The result of the extrapolation using an exponential form with $b = 130$ is shown by the (red) solid line. In the zero-winding number sector the data saturate much faster to the thermodynamic limit as is shown by the (black) horizontal line.](image-url)
The extrapolation to the thermodynamic limit $L \to \infty$ for fixed $L/\tau$ can be done in two ways. One way is to consider unmodified data for ever increasing values of $L/L/\tau$ and to extrapolate them using an exponential scaling law, $e^{-L/b}/\sqrt{L}$, [61] with a temperature-dependent fitting parameter $b$. In the quantum critical region the correlation length is directly proportional to $L/\tau$ (or inverse temperature), and direct measurements of the correlation length using the exponential decay of the single-particle density matrix indeed find that $\xi \approx 1.096(7)L/\tau$, see Fig. 4.3. It is thus expected that $b$ also scales with $L/\tau$ and the data are best fit with $b \approx 1.3L/\tau$. A typical example of the exponential extrapolation for the first non-zero Matsubara frequency at $L/\tau = 96$ is shown in Fig. 4.2. The other way is to collect statistics for correlation functions only in the zero winding number sector. It turns out that the second protocol is far more efficient in terms of system sizes required for reaching the asymptotic thermodynamic values, see Fig. 4.2. In the zero-winding sector the data are essentially in the thermodynamic limit already for $L/L/\tau = 2$, while unmodified data extrapolate to the same result within error bars only if the point $L/L/\tau = 4$ is included in the fit. We checked for consistency between the two protocols for a number of points but for the largest values of $L/\tau$ the simulation was done only in the zero winding sector using $L/L/\tau = 2$.

Quantum data were analyzed similarly. First, we calibrate the dependence of the correlation length $\xi$ on temperature at the critical point $(U/t)_{c} = 16.7424$ [20]. It is deduced from the exponential decay of the single-particle density matrix at large distances and is expected to increase $\propto 1/T$. The result of a linear fit shown in Fig. 4.3 leads to the asymptotic dependence $\xi(T) \approx 5.24(1)\beta t$ in units of the lattice constant $a$. The ratio $\xi/c\beta$, where $c$ is the sound velocity, is expected to be a universal characteristic of the quantum critical point, the same as $\xi/L/\tau$ in the classical J-current model. Using the value $c/a = 4.8(2)t$ determined in Ref. [2] we find that $\xi/c\beta = 1.09(4)$, in perfect agreement with the classical result for $\xi/L/\tau$. Given the exponential convergence of $\sigma(i\omega_{n})$ on $L$, we consider system sizes $L \approx 4\xi$.
Figure 4.3. The dependence of the correlation length on temperature at the critical point of (A) the two-dimensional Bose-Hubbard model and (B) the (2+1)-dimensional J-current model. As expected, at low temperature the dependence on $\beta = 1/T$ or $L_\tau$ is linear (solid line). Error bars are shown but are smaller than the symbol sizes.
(an equivalent of $L/L_\tau \approx 4.2$ for the classical system) for collecting unmodified data, and system sizes $L \approx 2\xi$ for collecting data in the zero-winding sector.

![Figure 4.4](image.png)

**Figure 4.4.** Extrapolating the conductivity in Matsubara representation to the universal zero-temperature limit for fixed $\omega_n/2\pi T = 7$.

### 4.3.2 Zero temperature extrapolation

Thermodynamic limit results for $\sigma(i\omega_n)$ have a smooth monotonic dependence on $L_\tau$ and can thus reliably be extrapolated to the universal $L_\tau \to \infty$ limit. We conjecture that the finite $L_\tau$ correction is captured by the leading irrelevant scaling field for the three-dimensional $U(1)$ universality class; its exponent $\omega$ was calculated and measured in a number of studies and estimates cluster around the field theoretical value $\omega \approx 0.80(2)$ [62]. In our analysis, we keep this exponent fixed at $\omega = 0.85$ since with this choice we observe that all fits are consistent with our error bars (if we include $\omega$ to the set of fitting parameters we find that its value is in the range $0.90 \pm 0.10$). When we perform a two parameter fit, $\sigma(i\omega_n/T, L_\tau) = \sigma(i\omega_n/T, \infty) + A_n/L_\tau^\omega$, see Fig. 4.4, we observe that the amplitudes
Figure 4.5. $A_n$ amplitudes deduced by fitting each Matsubara harmonic independently, see Fig. 4.4.

$A_n$ form a smooth curve obeying the law $A_n = A_0 + A n^\omega$ with the same exponent $\omega$, see Fig. 4.4, suggesting that the leading correction is indeed dominated by the correlation volume $(L/\tau)^3$. This allows us to perform a joint fit of all data points using $A_0$, $A$ and the universal conductivity as the only adjustable parameters to suppress point-to-point fluctuations and systematic error bars. The same protocol was applied to the quantum data.

4.4 Extreme sensitivity to the QCP position

As explained in the main text, the critical point of the J-current model is located at $K_c = 0.3330670(2)$ while the previous calculations in Ref. [55, 56] were done at $K = 0.33305$: i.e., on the insulating side of the transition point. This might seem to be an irrelevant difference but it does affect data for the universal conductivity to the extent that the shape of the universal $\sigma(i\omega_n)$ function is dramatically modified. As is clear from Fig. 4.4, the finite $L/\tau$ dependence is strong and large system sizes are required for a reliable extrapolation to
Figure 4.6. Statistics of winding numbers squared at $K = 0.33305$ as a function of system size. Instead of saturating to a constant, the data go through a maximum and start decaying visibly for $L = 128$. This is a clear signature of entering the insulating phase.

the universal limit. When simulations are done at $K = 0.33305$, the statistics of winding numbers squared (which is characteristic of current fluctuations at the largest scales) is significantly reduced relative to its critical behavior already for $L \approx 64$, see Fig. 4.6. If the lower values of $\sigma(i\omega_n, L_\tau)$ for large $L_\tau$ are then interpreted as a sign of convergence to the universal limit in the fitting procedure, the extrapolated values end up to be significantly lower than the correct ones.

4.5 J-current model

Results for the quantum-critical conductivity in the Matsubara representation $\sigma(i\omega_n)$ are shown in Fig. 4.7 for various values of $L_\tau$ along with the extrapolated zero-temperature limit. The universal conductivity quickly saturates to a plateau $\sigma(\infty) = 0.359(4)$ for $\omega_n/2\pi T > 6$, as is expected from Eq. (4.1).
Figure 4.7. (Color online) Thermodynamic limit data for the conductivity in Matsubara representation for increasing values of $L_\tau$, bottom to top. The universal result is obtained by extrapolating the data to the $L_\tau \to \infty$ limit (black filled circles).

In Fig. 4.8 we show the comparison between the universal data for $\sigma(i\omega_n)$ and predictions based on the holographic gauge/gravity duality. Clearly, the $T_B = T$ case is ruled out by the data. However, if the temperature scale for dynamics problems is renormalized relative to the thermodynamic temperature $T_B = T/\alpha$, as suggested in Ref. [54], then the theory contains an additional freedom for modifying the shape of the holographic curve by effectively rescaling the frequency axis by $\alpha$. For $\gamma = 1/12$ we find that $\alpha$ is close to 0.4. Unfortunately, this additional fitting parameter puts the test to the limit: given the benign shape of the imaginary frequency signal, much smaller error bars are required for furnishing a conclusive test—this is a well-known problem in the analytic continuation procedure when radically different functions in the real-frequency domain have very close shapes in the Matsubara domain. For example, a simple analytic expression, $\sigma(i\omega_n) = \sigma(\infty) + 1/P_3(\omega_n/T)$, where
$P_3(x)$ is the 3rd order polynomial, perfectly fits all our data, has all poles in the lower half-plane, but results in a dramatically different real-frequency signal, see inset in Fig. 4.8. Both outcomes suggest that transport is dominated by particle-like excitations. When we attempt other analytic continuation procedures such as the one used in the Higgs mode study [5], we find that the result is rather unstable, see Fig. 4.10. We thus conclude that the shape of the real frequency curve remains uncertain.

![Graph](image)

**Figure 4.8.** (Color online) Comparison between the numerical result for the universal conductivity in Matsubara space and holographic conductivity evaluated at complex frequencies. We consider only the largest possible value of the holographic parameter $\gamma = 1/12$ because it offers the best fit. The holographic curve can be made to fit the data much better if the temperature is scaled by a factor of 2.5. We also show the fit based on the 3rd order polynomial described in the text. The inset presents the possible universal real frequency conductivity curves obtained by analytical continuation of fitting functions.

### 4.6 Quantum model

Simulations of the quantum Bose-Hubbard model are far more demanding numerically resulting in larger error bars. Nevertheless, one can obtain reliable data for temperatures as
low as $\beta = 20/t$ in system sizes $L = 400$ which are required for eliminating finite-size effects. The result of extrapolation of the quantum model to the universal limit is shown in Fig. 4.9. As expected, the same result emerges from the quantum simulation, within error bars.

![Graph showing conductivity vs. $\omega/2\pi T$](image)

**Figure 4.9.** (Color online) Universal result for the conductivity in Matsubara representation from quantum Monte Carlo simulations for the Bose-Hubbard model. Temperature decreases from the bottom to the top, and the extrapolation to zero temperature is shown by black squares.

Unlike the classical model with discrete imaginary time direction, $\sigma(i\omega_n)$ for a quantum system is physically meaningful for all Matsubara frequencies and contains valuable information detailing the boundary between the universal and non-universal parts of the signal. We employ the formula

$$\sigma(i\omega_n) = \frac{2}{\pi} \int_0^\infty \frac{\omega_n}{\omega^2 + \omega_n^2} Re\sigma(\omega)d\omega,$$

(4.4)

to obtain the real part of conductivity on the real frequency axis, $\sigma(\omega)$. In Fig. 4.10 we show $\sigma(\omega)$ for the Bose-Hubbard model at low-temperature $T = 0.2t$ (for system size $L = 100$ and critical point parameters). At frequencies $\omega > 2\pi T \approx 1.3t$ the analytical continuation
procedure gets more stable and predicts, surprisingly, that the plateau at 0.35(5) extends up to $\omega \approx 15t$.

### 4.7 Experimental verification

There are prospects that temperatures are within reach of experiments with ultracold atoms in an optical lattice once new cooling schemes are implemented (this is a pressing issue for all proposals aimed at studies of strongly correlated states). One idea of measuring the optical conductivity is based on shaking the center of magnetic trap horizontally to create an effective “AC electric field” and particle currents. The energy absorbed by the system (it can be deduced by measuring the temperature increase) is proportional to $\text{Re}\sigma(\omega)$. An amplitude modulation of the lattice laser in combination with a similar energy absorption protocol has successfully been applied to study the Higgs amplitude mode in the Bose-Hubbard model\[3, 1\]. Alternatively, phase modulation was also proposed in Ref. [63] through the modulation of the position of a mirror reflecting the lattice laser beam, which allows us to measure $\omega^2\text{Re}\sigma(\omega)$. However, the low frequency signal may be masked by the prefactor $\omega^2$ if the experiment is set up this way.

### 4.8 Conclusions

In conclusion, we have constructed the universal conductivity in Matsubara representation by carefully extrapolating finite system size data to the thermodynamic limit $L \to \infty$ and then taking the $T \to 0$ limit. Our result $\sigma(\infty) = 0.359(4)\sigma_Q$ is the most accurate estimate of this quantity to date. The shape of the universal conductivity function in Matsubara representation was measured with reliable error bars for the first time and used to test the holographic theory\[11\]. The result of this comparison confirms that the theory has to include the possibility that the black brane temperature $T_B$ is renormalized relative to the thermody-
Figure 4.10. Real frequency conductivity of the Bose Hubbard system at $T/t = 0.2$ and $L = 100$. Both MaxEnt and consistent constraints analytical continuation methods [5] are tested.

dynamic temperature. For $T_B \approx 2.5T$ the holographic fit can be made marginally compatible with our data. An unambiguous proof of validity, which requires, however, more accurate data or models with weaker finite size effects, would constitute a major breakthrough in establishing the analytic continuation procedure for transport properties at quantum critical points [54]. On existing data, simple analytic expressions work as well. Finally, we also determine under what conditions $\sigma(\infty)$ can be measured with ultracold atoms in optical lattices.

Recently, a modified holographic theory which contains a new relevant term in the quantum gravity action is proposed in Ref. [12], and the authors claim the new theory is compatible to the numerical data without any rescaling on the temperature of the black hole. We plan to benchmark the new theory with more accurate numerical data in the future publications.
Part II

Impurity Problems at Quantum Criticality
CHAPTER 5
THE NOTION OF THE QUASIPARTICLE CHARGE

5.1 Introduction

If coupled to a ground-state many-body environment, an impurity—static or mobile, with or without internal degrees of freedom—gets dressed into a quasiparticle (polaron). The bare impurity normally carries well-defined intrinsic charges—discrete quantum numbers such as, e.g., the electric charge, particle number, or spin/angular momentum projection. (Some or all the intrinsic charges of the impurity can have zero values.) The charges of the polaron, however, are not supposed to be simply inherited from those of the bare impurity. Even more importantly, the latter charges do not have to be well-defined: In the presence of the environment charges, an impurity charge can become a bad quantum number.

The dichotomy of charge being either a good or bad quantum number is relevant not only to the properties of impurities/polarons. It applies to any kind of elementary excitations (quasiparticles). The famous example of elementary excitations characterized by well-defined particle charge are the quasi-particles/holes of Landau’s normal Fermi liquid. Two textbook examples of quasiparticles that cannot be characterized by a well-defined particle charge are phonons in superfluids and fermionic elementary excitations in superconductors.

In what follows, we will be mostly concerned with a static impurity, in which case (the expectation value of) the impurity charge is given by the integral of the expectation value of the charge-density distortion, \( \delta n(r) \), caused by the impurity (localized at the origin of the coordinates):

\[
q = \int \delta n(r) \, d^d r. \tag{5.1}
\]
When the bare impurity has its own non-zero charge, the latter should be added to the r.h.s. of Eq. (5.1). [For a mobile impurity, there is an analog of Eq. (5.1), where the integrand is the environment-impurity correlator.] The definition (5.1) implies a strict order of taking limits. The thermodynamic limit of infinite system size is taken first. This guarantees that $\delta n(r)$ vanishes at $r \to \infty$. Only then the infinite-range integration over $r$ is performed.

In the case when the charge of the dressed impurity is a good quantum number, $q$ takes on a certain integer value, which is generically insensitive to moderate changes in the strength $V$ of the coupling of the impurity to the medium. If the impurity charge is not a good quantum number, then the value of $q$ is $V$-dependent, and should be understood exclusively as an expectation—rather than eigen—value.

A peculiar situation emerges in the case when the charge, while being robust with respect to small changes of the coupling $V$, is not integer. Two characteristic examples are (i) the excitations on top of the Laughlin (fractional quantum Hall) ground state, and (ii) spinons (domain walls) in one-dimensional insulators with broken translation symmetry. For the simple reason that all the eigenvalues of the operator of the total number of particles are integer numbers, the fractional charge cannot be a good quantum number with respect to all possible measurements. In particular, any fractional charge is doomed to come as a fluctuating integer number within a measuring protocol—nowadays experimentally achievable with ultracold atoms in optical lattices—resulting in measuring the positions of all the particles in the system. Nevertheless, the robustness of the fractional charge in the above-mentioned examples is guaranteed by distinct topological properties of the wavefunctions and in this sense, does reveal universally good quantum numbers—corresponding topological charges.

In Chapter 6, we explore a mechanism of charge fractionalization, which does not involve topological quantum numbers and is due to rather special critical conditions taking place at a boundary quantum critical point (BQCP) of the transition between two states with well-defined charges [13]. For a static impurity, a necessary condition for the local charge to
be well-defined is vanishing charge compressibility. On the other hand, a necessary condition for the BQCP takes place is the absence of the charge gap. The two competing (!) conditions can be met in quantum-critical environments. For an impurity without internal degrees of freedom, the BQCP is achieved by fine-tuning the coupling strength $V$ to the critical value $V_c$. The same type of BQCP emerges for a (pseudo-)spin-1/2 impurity with an appropriate coupling to the charge density of the quantum-critical environment. Here no fine-tuning is required, since the symmetry between “spin-up” and “spin-down” states automatically guarantees that the impurity is at the BQCP, also implying that the local “magnetic” field—breaking the symmetry between “spin-up” and “spin-down” states—plays the role of the control parameter $(V - V_c)$ driving the system across the BQCP. On the approach to BQCP, the charge fractionalization comes in the form of a critically divergent halo carrying the charge $\pm 1/2$. At the transition point, there is only a microscopic core with half-integer charge. Across the BQCP, the sign of the halo flips, while the structure of the half-integer-charged core remains intact. Our study is based on Monte Carlo simulations with worm algorithm.

In Chapter 7, we show another exotic impurity physics, namely the charge of an attractive impurity can be divergent if the environment compressibility is ill-defined. This “trapping collapse” physics is relevant to the vacuum-superfluid or a generic superfluid–Mott-insulator quantum phase critical point. It is associated with a simple fundamental question we have addressed: how many repulsively interacting bosons can be localized by a potential well. We find that under rather generic conditions, for both weakly and strongly repulsive particles, in two and three dimensions—but not in one-dimension!—the potential well can trap infinitely many bosons. For example, even hard-core repulsive interactions do not prevent this “trapping collapse” phenomenon from taking place. For the weakly interacting/dilute regime, the effect can be revealed by the mean-field argument, while in the case of strong correlations the evidence comes from path-integral simulations. We also discuss the possibility of having a
transition between the infinite and finite number of trapped particles when strong repulsive inter-particle correlations are increased.

5.2 Effect of the environment on the impurity charge: Possible scenarios

With respect to a certain conserved Noether charge, corresponding environments fall into three categories: (i) environments with a charge gap in the excitation spectrum, (ii) gapless and compressible environments, (iii) gapless and incompressible environments and (iv) gapless environments with ill-defined compressibility. The first two (physically, very different) cases share the property of being unambiguous and simple in terms of the problem of impurity charge quantization.

In the presence of the charge gap, the response of the environment is quasi-perturbative. Therefore, the impurity charge is a good quantum number. Tuning the strength of the impurity-environment coupling can only cause a switch between two states with different charges at a certain “transition point” $V_c$. The transition, however, is merely nominal, because the charge gap protects the upper state from the decay, as long as the energy difference between the two states remains lower than the value of the gap, $\Delta$. Hence, for each “transition” point $V_c$, there are two associated end points: $V_+ > V_c$ and $V_- < V_c$; see Fig. 5.1. Normally, the charge-gapped environment is also characterized by well-defined particle/hole elementary excitations (carrying the charge $\pm 1$) with parabolic dispersion in the long-wave-limit; Mott insulator being a very typical example. In this case, the physics of the end point is universally captured by the single-particle Schrödinger equation. When $V$ approaches the end point $V_+$ from below, the charge-$(M+1)$ impurity experiences a dramatic evolution towards a loose dimer consisting of a well-localized charge-$N$ impurity and a weakly bound quasiparticle, the latter being described by the single-particle Schrödinger’s equation.
with a trapping boundary condition at the origin. At the end point $V_+$, the quasiparticle unbinds. A similar picture, up to interchanging $M + 1 \leftrightarrow M$ and replacing the weakly bound particle with a weakly bound hole, takes place when $V$ approaches the end point $V_-$ from above.

**Figure 5.1.** Schematic behavior of an impurity in a charge-gapped environment: The ground-state energy $E$ as a function of the impurity-environment interaction strength $V$, for two competing ground states. The value $V_c$ corresponds to a nominal transition between the state of the charge $M$ and the state of the charge $M + 1$. The values $V_-$ and $V_+$ correspond to the two end points (black dots) defined by the condition that the energy difference between the two competing states is exactly equal to the charge gap $\Delta$.

Within the context of quantization of the impurity charge $q$, the case (ii) is trivial. In Section 5.3, we prove a general statement that the charge of a static impurity cannot be a good quantum number as long as the charge-compressibility of the environment is finite. A compressible environment may or may not break the continuous symmetry associated with the intrinsic charge. The former case includes quantum ordered phases like the superfluid, while the latter case includes some gapless systems like the Luttinger liquids and Fermi liquids. These environments generate effective coupling terms mixing the states with different local charges, making the local charge a bad quantum number. When this happens, the
scenario of Fig. 5.1 would be simply replaced with the avoided-crossing (i.e., hybridization) one [see Fig. 5.2 (c)]. However, the upper branch can decay into the lower one due to the absence of the charge gap. As a result, in the absence of small parameters, the upper branch is either absent, or at least, significantly damped.

\[
\begin{align*}
E & = V q = M \\
E & = V q = M + 1
\end{align*}
\]

**Figure 5.2.** Schematic behavior of an impurity in a gapless environment with well-defined compressibility: The ground-state energy \( E \) as a function of the impurity-environment interaction strength \( V \). Three scenarios are possible: (a) Two quasiparticle states with quantized charge meet at a “first-order” phase transition point, similar to that of Fig. 5.1. The difference with the gapped environment here is that the upper states become decaying away from the critical point, the asymptotic metastability taking place in the limit \( V \to V_c \). (b) Two quasiparticle states with quantized charge are connected by a continuous phase transition—a boundary quantum critical point. The notion of an excited quasiparticle state is ill defined here. (c) The situation when the impurity charge is not quantized, which is expected for any compressible environment.

The case (iii)—a gapless and incompressible environment—is quite reach an intriguing. This kind of the environments can be found at some quantum critical points such as the superfluid–Mott-insulator QCP, paramagnet-antiferromagnet QCP. The zero compressibility of the environment allows the charge to be quantized. However, the quantized charge under the conditions of the case (iii) brings about an interesting problem of the nature of the transition between two states with different charges, as a function of the coupling strength.
The absence of the gap renders the upper state generically unstable with respect to the decay into the lower state. Nevertheless, the asymptotic metastability can take place in the limit $V \to V_c$ [see Fig. 5.2 (a)]. Such a scenario is characteristic, for example, for the (light) Fermi polaron [64, 65, 66]. The necessary and sufficient condition for the asymptotic metastability is the vanishing (in the $V \to V_c$ limit) ratio of the decay width of the upper state to the energy difference between the upper and lower states. As a result, the upper state is progressively well defined—and well separated from the lower state—when $V$ approaches $V_c$. The critical point is thus essentially the same as in the gapped case of Fig. 5.1: a doubly degenerate ground state of the impurity at $V = V_c$.

There also exists a scenario—observed in our recent numeric study [13]—when $V_c$ is the critical point of a fluctuational quantum phase transition for the impurity state, i.e., a boundary quantum critical point. With respect to each of the two competing ground states of the impurity, the BQCP plays the role of the end point. It is this scenario that will be addressed in detail in the chapter 6.

In a sense, the case (iv)—a gapless environment where the compressibility is ill-defined—proves to be even more exotic than the case (iii). The examples of such environments include vacuum-superfluid/generic superfluid–Mott-insulator phase transition point (at any dimensions) and vacuum-Fermi liquid transition point ($d < 3$). The charge of an attractive impurity in this case translates into the number of bounded bosons/fermions in the effective potential well. The charge number for a well in the fermionic systems (including the $d = 1$ vacuum-superfluid QCP, which has an effective fermionic description) has to be finite and should be quantized due to the Pauli exclusion principle. However, the charge number for a potential well in the two- and three-dimensions bosonic systems can be divergent, regardless of the strong repulsion between bosons. We discuss this “trapping collapse” physics in the Chapter 7.
5.3 Absence of charge quantization for a static impurity in a charge-compressible environment

In this section, we will prove a theorem, which states that the impurity charge will be finite but not quantized if the environment has a finite charge-compressibility.

Without loss of generality, we will be assuming that the charge in question is associated with the number of particles of the environment, and that we are dealing with a continuous-space system, so that the static impurity is represented by an external potential $U(r)$:

$$H_{\text{imp}} = \int U(r)n(r)\,d^dr,$$  \hfill (5.2)

where $n(r)$ is the operator of the number density.

The statement of the appendix title immediately follows from the general relation

$$\frac{\delta q}{\delta U(r)} \bigg|_{U=0} = \kappa,$$  \hfill (5.3)

where,

$$\kappa = \frac{\partial n}{\partial \mu} \quad \text{(in the grand-canonical variables)}$$  \hfill (5.4)

is the compressibility which is well-defined; the partial derivative being taken in the grand-canonical variables, i.e., at fixed volume and temperature. We thus want to derive (5.3).

Consider a cubic $d$-dimensional system of linear size $L$, at a small but finite temperature $T$. The compressibility of the system is given by

$$\kappa_L \equiv \kappa_L(\mu,T) = \left( \frac{\partial n}{\partial \mu} \right)_{L,T} = \frac{\langle (\Delta N)^2 \rangle}{TL^d}.$$  \hfill (5.5)

In this formula, the first equality is nothing but the definition, while the second equality—with $\langle (\Delta N)^2 \rangle$ being the variance of the total number of particles—is a straightforward implication of the definition, coming directly from the grand canonical distribution.
A subtlety arises when (5.5) is used—in particular, in first-principle numeric simulations—to extract the thermodynamic value $\kappa_0$ of the ground-state compressibility. Here the limits $T \to 0$ and $L \to \infty$ have to be taken under the condition of $TL^d \to \infty$, or equivalently, in the strict order (from left to right):

$$\kappa = \lim_{L \to \infty} \kappa_L, \quad \kappa_0 = \lim_{T \to 0} \kappa.$$  \hspace{1cm} (5.6)

The crucial role of the requirement

$$TL^d \to \infty,$$  \hspace{1cm} (5.7)

fixing the order of limits in (5.6), is clear from the very structure of the rightmost expression in Eq. (5.5). The effects of finite-size quantization get completely eliminated only in the limit of diverging variance of the particle-number fluctuations, and the condition (5.7) is necessary and sufficient for this to happen.

Similarly, the definition of the impurity charge, Eq. (5.1), is insensitive to the finite-size effects, if the grand canonical ensemble is used and the ground-state thermodynamic limit is taken under the constraint (5.7), or equivalently, the order of limits is exactly the same as in (5.6). Here the requirement (5.7) guarantees the absence of the spurious contributions to the integral (5.1) coming from the distances of the order of the system size.

Using Kubo formula, for the variational derivative in the l.h.s. of (5.3) we have

$$\left. \frac{\delta q}{\delta U(r)} \right|_{U=0} = \int K(r-r', \tau) d^d r' d\tau$$  \hspace{1cm} (5.8)

$$K(r, \tau) = \langle [n(0,0) - \bar{n}] [n(r,\tau) - \bar{n}] \rangle,$$  \hspace{1cm} (5.9)

where $n(r, \tau)$ and $\bar{n}$ are, respectively, the Matsubara operator and the expectation value of the number density. The integration over $r'$ converts the number density operator into
the operator of the total number of particles (here we also use $\bar{n}L^d = \bar{N}$ and the fact that $N(\tau) \equiv N$, since the operator $N$ commutes with the Hamiltonian):

$$\int K(\mathbf{r} - \mathbf{r}', \tau) \, d^d r' = \langle [n(0, 0) - \bar{n}] [N - \bar{N}] \rangle. \quad (5.10)$$

The $\tau$-independence of the r.h.s. of (5.10) trivializes the integration over $\tau$ in (5.8). The last simple step we need to take to convert the r.h.s. of (5.8) into the r.h.s. of (5.5) is the observation that translation invariance allows us to replace $[n(0, 0) - \bar{n}]$ in (5.10) with $(N - \bar{N})/L^d$. 
6.1 Introduction

6.1.1 The halon

The halon is a special critical state of an impurity in a quantum-critical environment. The hallmark of the halon physics is that a well-defined integer charge gets fractionalized into two parts: a microscopic core with half-integer charge and a critically large halo carrying a complementary charge of $\pm 1/2$. The halon phenomenon emerges when the impurity–environment interaction is fine-tuned to the vicinity of a boundary quantum critical point (BQCP), at which the energies of two quasiparticle states with adjacent integer charges approach each other.

The first example of the halon is discovered in the study of a static impurity in a two-dimensional superfluid–Mott-insulator quantum critical system [13]. Specifically, we performed worm-algorithm simulations of the standard Bose-Hubbard model on the square lattice, with the impurity (a trapping center) located at the site $i = 0$:

$$H = - \sum_{\langle ij \rangle} b_i^\dagger b_j + \frac{U}{2} \sum_i n_i(n_i - 1) - \mu \sum_i n_i + V n_{i=0}.$$ (6.1)
Here $b_i^\dagger$ and $b_i$ are, respectively, bosonic creation and annihilation operators on the site $i$; the symbol $\langle \ldots \rangle$ stands for nearest-neighbors; $U$ is the on-site interaction in units of hopping amplitude, the latter being set equal to unity. The simulations were performed at unit filling factor, setting $U$ and the chemical potential, $\mu$, equal to their critical values, $U_c = 16.7424(1)$, $\mu_c = 6.21(2)$ [19, 2, 20]. We observed a scenario of Fig. 5.2 (b), with a peculiar critical behavior of the charge distribution, Fig. 6.1, which is likely to be generic for all fluctuational transitions between the two charge-quantized impurity states. When the center strength $V$ approaches its critical value $V_c = 6.86(8)$, the integer impurity charge separates into a short-ranged half-integer core and a large halo carrying the complementary charge of $\pm 1/2$. The sign of the halo changes across the transition and the radius of the halo, $r_0$, diverges on the approach to $V_c$, following the critical law

$$r_0 \propto |V - V_c|^{-\tilde{\nu}}, \quad \tilde{\nu} = 2.33(5). \quad (6.2)$$

One can also show [13] (corresponding analysis is rendered in our Sec. 6.3) that the exponent $\tilde{\nu}$ controls some other critical properties; for example, the nonperturbative contribution to the energy:

$$E(V_c) - E(V) \propto |V - V_c|^{\tilde{\nu}}, \quad (6.3)$$

as well as the power-law charge distribution in the inner part of the halo:

$$|\delta n(r)| \propto \frac{1}{r_0^{2-s}r^s}, \quad s = 1 + 1/\tilde{\nu} \quad (r \ll r_0). \quad (6.4)$$

We presented the following argument explaining why the exact half-integer quantization of the halo charge—and, correspondingly the charge of the core—follows from the very fact of existence of the halo with diverging size $r_0$. The relativistic long-range physics of the U(1) quantum criticality is particle-hole symmetric. Therefore, there should exist two halo
solutions that differ only by the sign of the density distortion. In terms of these two solutions, the net change of the impurity charge across the transition equals (plus/minus) two times the absolute value of the halo charge. Since the change of the net charge is ±1, the halo charge has to be ±1/2. More generally, the emergent particle-hole symmetry at $V \to V_c$ implies the self-duality of the boundary quantum phase transition.

![Figure 6.1. Emergence of the halon. Tuning the impurity-environment interaction strength $V$ drives the quasiparticle state across a boundary quantum critical point $V_c$. The integer impurity charge separates into a short-ranged half-integer core and a large halo carrying the complementary charge of ±1/2. When $V$ crosses the transition point, the charge in the core remains the same, while the charge of the halo changes its sign, resulting in a ±1 change in the net quasiparticle charge.](image)

### 6.1.2 The spin-1/2 Bose Kondo model

In this section, we propose an effective model to describe the halon physics in a $U(1)$ quantum critical environment as the Hamiltonian (6.1).

Consider a model where a static (pseudo-)spin-1/2 impurity couples to the $U(1)$ Wilson–Fisher conformal bosonic field by the following interaction Hamiltonian.

$$H_{\text{BK}} = \gamma [\hat{S}_+ \hat{\psi}(r = 0) + \hat{S}_- \hat{\psi}^\dagger(r = 0)] + h_z \hat{S}_z.$$ (6.5)
Here $\hat{\psi}(\mathbf{r})$ is the field operator, $\hat{S}_z$ is the $z$-component of the operator of spin, and $\hat{S}_- +$ and $\hat{S}_-$ are corresponding ladder operators.

The coupling (6.5) preserves the global $U(1)$ symmetry of the conformal field theory—with the global $U(1)$ transformation involving corresponding rotation of the spin variables in the $xy$ plane—leading to the conservation of the Noether’s charge

$$Q = \hat{S}_z + \int d^d r \, \hat{\psi}^{\dagger} \hat{\psi}. \quad (6.6)$$

The $U(1)$ Wilson–Fisher conformal bosonic field theory is particle-hole symmetric. At $h_z = 0$, the coupling (6.5) respects this symmetry as well, with the particle-hole transformation accompanied by flipping the spin variables with respect to the $z$-axis.

As long as we accept the concept of universality of critical phenomena, we have to conclude that the model (6.5) captures the universality class of the halon physics of the Hamiltonian (6.1). An advantage of the model (6.5) compared to (6.1) is that the particle-hole symmetry [emergent in the model (6.1) in the long-wave limit at $U = U_c$, $\mu = \mu_c$, and $V \to V_c$] now takes place at the microscopic level at $h_z = 0$, meaning that the latter condition defines the halon BQCP. The correlation length of the critical response to small $h_z$,

$$\xi_z \propto |h_z|^{-\nu_z}, \quad (6.7)$$

defines the halo radius:

$$\xi_z \equiv r_0, \quad \nu_z \equiv \tilde{\nu}. \quad (6.8)$$

At the halon BQCP, there is yet another exponent, independent of $\tilde{\nu}$ and associated with the correlation length of the response to the local $U(1)$-breaking field. In terms of the model
(6.5), corresponding term, $h_\perp \hat{S}_x$ or $h_\perp \hat{S}_y$, is generated by coupling the spin to the magnetic field in the $xy$-plane. For the associated correlation length we then have

$$\xi_\perp \propto |h_\perp|^{-\nu_\perp}.$$  

(6.9)

The other critical exponents can be related to $\nu_z$ and $\nu_\perp$ by general arguments of the theory of critical phenomena.

The model (6.5) is known in literature [67], along with other models of impurities coupled to a bulk critical environment [68, 69, 70, 71, 72]. However, the relevance of the model to the halon physics was realized only recently, by Whitsitt and Sachdev in Ref. [73], and by us in the present paper. Whitsitt and Sachdev employed the model for renormalization-group calculations, yielding, in particular, the values of the exponents $\nu_z$ and $\nu_\perp$. In what follows, we present the results of worm-algorithm simulations of a microscopic counterpart of (6.5) featuring the built-in $U(1) \times Z_2$ symmetry at the critical point $h_z = 0$. In particular, we demonstrate (by showing that $\nu_z = \tilde{\nu}$ within the error bars) that the spin-1/2 impurity model captures the universality class of the BQCP of the model (6.1).

Kondo-type models, where a spin-1/2 impurity couples to this or that gapless charge-conserving environment—most notably, the bosonic one, giving rise to the family of Bose Kondo models [68, 69, 70, 71, 67]—are particularly suited (while being also interesting in a broader context) for addressing the properties of the medium with respect to the quantization of the impurity charge. In the absence of magnetic field applied to the spin-1/2 impurity: $h_z = 0$, the state of the impurity naturally corresponds to the critical point $V_c$ of the transition between two charge-quantized states (if any, see Fig. 5.2.) The absence of charge quantization, Fig. 5.2 (c), corresponds to the Kondo effect, when the impurity entangles with the environment to form a singlet-type state. The case of Fig. 5.2 (a) corresponds to the absence of the Kondo effect. Here the impurity is essentially disentangled from the bulk of
the system. In terms of the Kondo effect, the critical situation of Fig. 5.2 (b) is marginal. In a sense, the effect does take place at $h_z = 0$, when the spin of the impurity entangles with the whole system. However, the resulting state is critical and thus is dramatically affected by a finite $h_z$: The characteristic length of the entanglement region—the halo—becomes finite. Note also that the $\pm 1/2$ charge of the halo naturally follows from the first term of Eq. (6.6), and the self-duality of the halon phase transition is seen at the microscopic level by the $h_z \rightarrow -h_z$ symmetry.

In the renormalization group language applied to Bose Kondo models (6.5), the three scenarios of Fig. 5.2 are related to the known three different types of the infrared fixed points for the running coupling constant $\gamma$ (at $h_z = 0$) [74]. The weak-coupling fixed point $\gamma = 0$, the intermediate-coupling fixed point $\gamma > 0$, and the strong-coupling fixed point $\gamma = \infty$ represent the cases (a), (b), and (c), respectively.

### 6.1.3 O($N$) quantum rotor model

The Bose Hubbard model (6.1) provides a prototypical model for the halon effect. However, the halon physics can be found in a broad class of quantum critical environments. One possible generalization is considering the static impurity in the $O(N)$ quantum rotor model for arbitrary $N \leq 2$. Notice the $O(2)$ quantum rotor model captures the universality class of the quantum phase transition of the Bose Hubbard Hamiltonian while encoding the particle-hole symmetry at the microscopic scale:

$$\hat{H}_R = \frac{g}{2} \sum_i \hat{L}_i^2 - J \sum_{\langle i,j \rangle} \hat{\mathbf{n}}_i \cdot \hat{\mathbf{n}}_j.$$ \hspace{1cm} (6.10)

The rotor leaving on the site $i$ of a certain lattice is described by the operator $\hat{\mathbf{n}}_i$ of a unit vector in a generalized $N$-dimensional coordinate space. Corresponding momentum $\hat{\mathbf{p}}_i$ is introduced by the commutation relations
\[ \left[ \hat{n}_i^{(\alpha)}, \hat{p}_i^{(\beta)} \right] = i\delta_{\alpha,\beta}, \quad (6.11) \]

with \( \alpha, \beta = 1, 2, \ldots, N \) labelling the components. The rotor angular momenta \( \hat{L}_i \) are the generators of the \( N \)-dimensional rotational symmetry group \( O(N) \); they have \( N(N - 1)/2 \) independent components:

\[ \hat{L}_i^{(\alpha\beta)} = \hat{n}_i^{(\alpha)} \hat{p}_i^{(\beta)} - \hat{n}_i^{(\beta)} \hat{p}_i^{(\alpha)}. \quad (6.12) \]

The first term in the Hamiltonian (6.10) is the inner product of two angular momentum operators and plays the role of the kinetic energy of the rotors with \( 1/g \) the rotor moment of inertia, while the second term (with \( J > 0 \)) is the “ferromagnetic” coupling between the rotor orientations on neighboring sites.

While elementary quantum rotors do not exist in nature, the universality of quantum critical phenomena renders the model (6.10) relevant to a broad class of experimentally realizable systems [25]. As we already mentioned, the \( N = 2 \) case captures the universality class of the superfluid–Mott-insulator transition in the Bose Hubbard (and similar) models. Moreover, in the limit of large integer filling factor, the Bose Hubbard model becomes microscopically equivalent to the \( O(2) \) rotor model. In this case, \( \hat{n}_j^{(1)} \) and \( \hat{n}_j^{(2)} \) are related to the bosonic creation operator by \( \hat{b}_j^{\dagger} \propto (\hat{n}_j^{(1)} + \hat{n}_j^{(2)})/2 \). The angular momentum operator \( \hat{L}_j \) now has only one independent component \( \hat{L}_j^{(12)} \). In terms of the underlying Bose Hubbard model at large integer filling factor, this operator corresponds to the deviation of the on-site occupation number from its expectation value. In the case of \( N = 3 \), the quantum rotor model describes the spin-1/2 “dimerized” antiferromagnets, where each unit cell contains even number of spins. In these systems, the angular momentum \( \hat{L}_j \) has three components corresponding to three local magnetization projections.

The type of the ground state of the model (6.10) is controlled by the dimensionless parameter \( g/J \). At \( g/J \gg 1 \), the first term dominates, leading the system to a quantum “paramagnetic” state. On the other hand, the interaction term in Eq. (6.10) is minimized
by aligning the rotors. This term dominates at \( g/J \ll 1 \), bringing the system to a “magnetically” ordered state with \( \langle n \rangle \neq 0 \). The competition between the two states leads to a continuous quantum phase transition at a certain critical point \( (g/J)_c \). The model (6.10) is thus representative of the \( O(N) \) quantum criticality (known to have emergent Lorentz symmetry). In what follows, we will be assuming that the ratio \( g/J \) is kept precisely at \( (g/J)_c \).

A static spinless impurity responsible for the halon effect in the quantum rotor model is introduced in a direct analogy with the Bose Hubbard model (6.1): The impurity has to couple to a Noether charge density operator. Without loss of generality, we assume that corresponding local field is applied to one of the components of the orbital angular momentum, say \( \hat{L}^{(12)} \), on the site \( i = 0 \):

\[
\hat{H}_R \rightarrow \hat{H}_R + V \hat{L}^{(12)}_{i=0}.
\]

This term breaks the global symmetry from \( O(N) \) to \( O(2) \times O(N - 2) \), where the \( O(2) \) symmetry guarantees that the total \( (12) \)-component of the angular momentum,

\[
Q = \sum_i \hat{L}^{(12)}_i,
\]

is still a conserved charge.

Increasing the strength \( V \) of the local field causes the trapped charge to change. If the charge is quantized—and our first-principle simulations show that it is quantized at least for \( N = 2 \) and \( N = 3 \), boundary quantum phase transitions occur at certain \textit{finite} critical values of \( V \), while a certain finite interval around the point \( V = 0 \) corresponding to zero trapped charge. The \( Z_2 \) (particle-hole) symmetry of the rotor model guarantees the equivalence between the positive and negative critical values of \( V_c \), but tells nothing about the critical
values themselves. A more interesting situation takes place when one introduces a spin-1/2 impurity [cf. Eq. (6.5)]:

$$\hat{H}_R \rightarrow \hat{H}_R + \gamma \left[ \hat{S}_+ \hat{n}_{i=0}^-(\downarrow) + \hat{S}_- \hat{n}_{i=0}^+(\uparrow) \right] + h_z \hat{S}_z,$$

(6.15)

where

$$\hat{n}_{i}^{(\pm)} = (\hat{n}_{i}^{(1)} \pm i\hat{n}_{i}^{(2)})/2$$

(6.16)

are the ladder operators for the (12)-component of the angular momentum:

$$[\hat{n}_{i}^{(\pm)}, \hat{L}_{i}^{(12)}] = \mp \hat{n}_{i}^{(\pm)}.$$  

(6.17)

In this model, the global Noether charge—the analog of (6.14)—becomes

$$Q = \hat{S}_z + \sum_i \hat{L}_i^{(12)},$$

(6.18)

and the Z$_2$ (particle-hole) symmetry guarantees that $h_z = 0$ is the BQCP corresponding to the transition between the states with $Q = +1/2$ and $Q = -1/2$.

In the long-wave length limit, the effective field theory for the $d$-dimensional quantum rotor model at the quantum critical point is a $(d + 1)$-dimensional critical $\phi^4$ field theory, where $\phi$ is a continuous O($N$) vector field. This allows us to use the well-established critical $\phi^4$ field theory to study the halon physics in the rotor model.

### 6.2 Upper critical dimension for the halon effect

The mapping of the halon problem onto the Bose Kondo problem is very convenient for establishing the upper critical dimension for the halon effect. Here we perform the calculation
for the O(N) quantum critical environment by rendering the known results for the spin-1/2 impurity.

Beyond the critical dimension, the physics is perturbative, see Fig. 5.2 (a). The condition for this picture to take place is

\[
\lim_{h_z \to 0} \frac{\Gamma(h_z)}{h_z} \to 0, \quad (6.19)
\]

where \(\Gamma(h_z)\) is the decay width of the upper branch as a function of the energy splitting \(h_z > 0\). Without loss of generality, we assume that our microscopic Hamiltonian is the quantum rotor model (6.15), and use the Fermi Golden rule in the interaction picture

\[
\Gamma = \int_{-\infty}^{\infty} \langle \dot{H}_{\text{imp}}(0) \dot{H}_{\text{imp}}(t) \rangle \, dt, \quad (6.20)
\]

\[
\dot{H}_{\text{imp}}(t) = e^{i h_z t} \dot{S}_+ \hat{n}_{i=0}^{(-)}(t) + e^{-i h_z t} \dot{S}_- \hat{n}_{i=0}^{(+)}(t). \quad (6.21)
\]

We thus see that \(\Gamma(h_z)\) is given by the frequency-\(h_z\) Fourier component of the temporal correlator (being interested in the \(h_z \to 0\) limit, we use the universal long-time asymptotic form of the correlator)

\[
\langle T \hat{n}_{i=0}^{(-)}(0) \hat{n}_{i=0}^{(+)}(t) \rangle \propto \frac{1}{|t|^{d+z-2+\eta}}. \quad (6.22)
\]

Here \(z = 1\) is the dynamic exponent and \(\eta\) is the anomalous critical exponent of the \((d + 1)\)-dimensional O(N) universality class. (The exponent \(\eta\) is nonzero only below the upper critical dimension \(d = 3\).) Performing the Fourier integral then gives

\[
\Gamma(h_z) \sim \gamma^2 h_z^{d-2+\eta}. \quad (6.23)
\]

We conclude that the upper critical dimension for the halon physics is \(d = 3\), the same as for the quantum critical environment: Equation (6.23) becomes meaningful—consistent with (6.19)—at \(d > 3\).
While clearly characterizing the situation at \( d > 3 \), Eq. (6.23) leaves open the question of what happens at \( d = 3 \). Here the r.h.s. of (6.23) is directly proportional to \( h_z \), meaning that as long as \( \gamma \) is small enough, we have \( \Gamma \ll h_z \), which seems to justify using Fermi Golden rule, but the result we get this way is not consistent with (6.19) thus calling for a more delicate analysis.

The analysis clarifying the situation in three dimensions has been performed in Refs. [68, 67, 73] by the methods of perturbative renormalization group. The perturbative renormalization group treatment for a generic Bose Kondo model has been developed in Ref. [68, 69, 67]. The method is based on the dimensional regularization \( d = 3 - \epsilon \). It becomes controllably accurate at \( \epsilon \to 0 \), which is the case of our interest. The results of Refs. [68, 67, 73] show that the low-energy theory at the \( Z_2 \) symmetric point \( h_z = 0 \) is controlled by an infrared fixed point described by a Bose Kondo impurity model with an effective coupling strength \( \gamma_* \sim \epsilon \). At \( \epsilon = 0 \), the effective coupling \( \gamma_* \) vanishes, meaning that the (renormalized) impurity and the environment are completely decoupled, which corresponds to the scenario Fig. 5.2 (a). Hence, the situation in three dimensions is essentially the same as at \( d > 3 \).

When \( \epsilon > 0 \), the infrared fixed point of the perturbative RG treatment has an intermediate coupling strength \( 0 < \gamma_* < \infty \), suggesting a nontrivial BQCP at \( d = 2 \). Although \( \epsilon \) is not a small parameter here, the leading-order calculation seems to properly capture the qualitative physics of the system. Furthermore, comparison to our unbiased Monte Carlo results demonstrates that the third-order \( d = 3 - \epsilon \) calculation performed recently by Whitsitt and Sachdev [73] is quite accurate in reproducing the boundary quantum critical exponents.

### 6.3 General properties of the halon

In this section, we will discuss some general properties of the halon. Without loss of generality, we will be using the language of the Bose Kondo model (6.5) in the vicinity of the BQCP.
Our starting point is the hyperscaling ansatz of the BQCP. As explained in the introduction, the BQCP is controlled by two independent boundary quantum critical exponents $\nu_z$ and $\nu_\perp$. The former is the scaling dimension of the $\mathbb{Z}_2$-symmetry-breaking field $h_z$, the latter is the scaling dimension of the local $U(1)$-symmetry-breaking field $h_\perp$, which is coupled to $\hat{S}_x$ (or $\hat{S}_y$) of the impurity. In the absence of dangerously irrelevant terms, one can write down the hyperscaling ansatz in the vicinity of the BQCP for the singular part of free energy

$$F_s = b^{-z}\Phi(h_z b^{1/\nu_z}, h_\perp b^{1/\nu_\perp}, ...),$$

for an arbitrary rescaling parameter $b$, which rescales the spatial variable as $x \to x/b$ and imaginary time variable as $\tau \to \tau/b^z$. Here, the dynamic exponent $z > 0$ is the scaling dimension of time variable of the bulk quantum criticality. In the following discussion, we will assume that $z = 1$ because a bosonic system with (emergent) particle-hole symmetry normally already implies (emergent) Lorentz invariance. However, certain edge cases (say, Lifshitz points) may have $z > 1$, and our main results can also be easily adapted.

In the above hyperscaling ansatz, we assume that both the system size $L$ and the inverse temperature $\beta = 1/T$ are much larger than the correlation length $\xi_{z,\perp}$ (as in Eq. (6.7) or Eq. (6.9)). Physically, it means that one needs to take the thermodynamic limit before approaching the BQCP as $h_z, h_\perp \to 0$.

### 6.3.1 Halon Dynamics

We first explore the halon dynamics, which corresponds to the local spin dynamics of the Bose Kondo model. For convenience, we will mainly work with the correlation functions in the imaginary time/Matsubara frequency. They can be analytically continued to the real-frequency retarded response functions, which can be directly observed in experiments.

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1Here and in what follows we adopt a convention of omitting regular parts in critical relations
We consider two trajectories approaching the BQCP. One is \((h_z \to 0, h_\perp = 0)\), and the other is \((h_z = 0, h_\perp \to 0)\). Along these two trajectories, the characteristic length scales are \(\xi_z\) and \(\xi_\perp\), respectively. For each trajectory, there is only one relevant term in the hyperscaling hypothesis Eq. (6.24) so that we can choose the rescaling parameter \(b\) to be the corresponding correlation length itself.

For the spin-1/2 impurity in the XY Bose Kondo model, there are two independent spin correlation functions,

\[
\chi_\alpha(\tau) \equiv \langle \delta \hat{S}_\alpha(\tau) \delta \hat{S}_\alpha(0) \rangle,
\]

(6.25)

where \(\alpha\) can be either longitudinal index \(z\) or transverse index \(\perp\), and \(\delta \hat{S}_\alpha \equiv \hat{S}_\alpha - \langle \hat{S}_\alpha \rangle\) is the spin fluctuation operator.

The Matsubara-frequency-dependent local susceptibility is defined as the Fourier component of the correlation function \(\chi_\alpha(i\omega_n) = \int_0^\beta \chi_\alpha(\tau) exp(-i\omega_n\tau) d\tau\). The singular part of the static local susceptibility can be derived from the hyperscaling ansatz (6.24), \(\chi_\alpha(i\omega_n = 0) = \frac{\partial^2 F_s}{\partial h_\alpha^2} \sim \xi_\alpha^{2/\tilde{\nu}_\alpha - 1}\), where the correlation length \(\xi_\alpha \sim |h_\alpha|^{-\tilde{\nu}_\alpha}\) diverges when approaching to the BQCP. This equation implies that the correlation function scales as

\[
\chi_\alpha(\tau) \sim \frac{1}{\xi_\alpha^{2-2/\tilde{\nu}_\alpha}} \Psi_\alpha(\tau/\xi_\alpha) .
\]

(6.26)

Since the short time dynamics \(\tau \ll \xi_\alpha\) should be independent of the finite correlation length, we conclude that

\[
\Psi_\alpha(x) \to x^{2/\tilde{\nu}_\alpha - 2}, \quad x \ll 1,
\]

(6.27)

or

\[
\chi_\alpha(\tau) \sim \frac{1}{\tau^{2-2/\tilde{\nu}_\alpha}}, \quad \tau \ll \xi_\alpha .
\]

(6.28)

Since the correlation function can not diverge, this equation also imposes a lower bound for the boundary critical exponent \(\tilde{\nu}_\alpha > 1\).
On the other hand, in the long-time limit $\tau \gg \xi_\alpha$, the correlation functions should be dictated by a very simple perturbative physics. Indeed, the boundary-critical fluctuations are suppressed, leaving no room for non-linear effects. The correlation function thus demonstrates a generic linear response identical—up to the global amplitude—to the response caused by replacing the spin impurity Hamiltonian (6.5) with a weak local perturbation,

$$H_{\text{pert}} = \tilde{V} \hat{n}_{r=0}. \tag{6.29}$$

Hence, at the limit $\tau \gg \xi_\alpha$, the spin-spin correlation functions of the Bose Kondo model can be mapped to the density-density correlation functions of the weak local perturbation problem, so that

$$\chi_z(\tau) \propto \langle \hat{n}_{r=0}(\tau) \hat{n}_{r=0}(0) \rangle |_{H_{\text{pert}}}, \tag{6.30}$$

and

$$\chi_\perp(\tau) \propto \langle T \hat{\psi}_{r=0}(\tau) \hat{\psi}_{r=0}(0) \rangle |_{H_{\text{pert}}}. \tag{6.31}$$

The r.h.s of (6.30) is known to demonstrate a power-law behavior $\sim 1/\tau^{2d}$ because the scaling dimension of the particle number density—or the Noether charge density—is $d$, which coincides with its canonical dimension. On the other hand, the r.h.s of (6.31) is the order parameter correlation of the bulk, $\sim 1/\tau^{d-1-\eta}$, where $\eta$ is the anomalous scaling dimension of the order parameter field. These tails fix the long-time limit of the universal behavior of $\Psi(x)$,

$$\Psi_z(x) \to 1/x^{2d} \quad \text{and} \quad \Psi_\perp(x) \to 1/x^{d-1-\eta}, \quad x \gg 1. \tag{6.32}$$

In experiment, a more relevant observable is the the retarded dynamic susceptibilities $\tilde{\chi}_\alpha(\omega)$ which depends on the real frequency. This quantity can be obtained by analytically continuing the Matsubara-frequency correlation function $\chi(i\omega_n)$ to real-frequencies,

$$\tilde{\chi}_\alpha(\omega) = \chi_\alpha(i\omega_n \to \omega + i0^+). \tag{6.33}$$
Using this relation, the scaling hypotheses for the dynamic susceptibilities are implied by Eq. (6.26),
\[ \tilde{\chi}_\alpha(\omega) \sim \xi_\alpha^{2/\bar{\nu}_\alpha - 1} \Phi_\alpha(\omega \xi_\alpha). \tag{6.34} \]

The universal functions \( \Phi_\alpha \) in the limits \( x \ll 1 \) and \( x \gg 1 \) are known as
\[ \Phi_\alpha(x) \sim x^{1-2/\bar{\nu}_\alpha}, \quad x \gg 1, \tag{6.35} \]

and
\[ \Phi_z(x) \sim x^{2d-1}; \quad \Phi_\perp(x) \sim x^{d-2-\eta}, \quad x \ll 1. \tag{6.36} \]

We now investigate the transverse dynamic susceptibility \( \tilde{\chi}_\perp \) in more detail. Since the impurity can not fluctuate faster than the environment\[^75, 74\], the exponent of the universal function \( \Phi_\perp(x) \) in the limit \( x \ll 1 \) should be larger than that in the limit \( x \gg 1 \), namely \( d - 2 - \eta > 1 - 2/\bar{\nu}_\perp \). In the most interesting case of \( d = 2 \), it imposes an upper bound for the boundary exponent \( \bar{\nu}_\perp \leq 2/(1 + \eta) < 2 \) where \( \eta > 0 \) holds for any nontrivial bulk quantum criticalities. For example, as we will show in the next section, the exponent for the \( O(2) \) bulk quantum criticality is numerically calculated to be \( \bar{\nu}_\perp = 1.15(3) \), which is consistent with this upper bound. The universal dynamic susceptibility is illustrated in Fig. 6.2 (right). On approach to the limit \( \omega \to 0 \), the universal function diverges as \( 1/\omega^\eta \). On the other hand, in the high frequency limit \( \omega \to +\infty \), the universal function decays as \( 1/\omega^{2/\bar{\nu}_\perp - 1} \). The crossover from the low-frequency limit to the high-frequency limit occurs around \( \omega \sim 1/\xi_\perp \).

Interestingly, the longitudinal dynamic susceptibility is radically different from the transverse one. In \( d = 2 \), its low frequency part behaves as \( \omega^3 \), i.e., does not diverge in the \( \omega \to 0 \) limit, and its high frequency part behaves as \( \omega^{1-2/\bar{\nu}_z} \). According to our recent numerical simulations for the \( O(2) \) bulk quantum criticality \[^13\], we find the exponent \( \bar{\nu}_z = 2.33(5) > 2 \). As a result, the longitudinal dynamic susceptibility develops a pseudo platform \( \omega^{0.14(2)} \) at
the high frequency limit. These features are illustrated in Fig. 6.2 (left). The crossover from
the low-frequency limit to the high-frequency limit again occurs around $\omega \sim 1/\xi_z$.

For both dynamic susceptibilities, the behavior near the intermediate frequency $\omega \sim 1/\xi_\alpha$—which is closely related to the quasiparticle pole information of the halon excitation—remains unclear. We plan to address this important issue in the near future.

\begin{figure}[h]
\centering
\begin{tikzpicture}
\begin{axis}[
    title={$\tilde{\chi}_z(\omega)$},
    xlabel=$\omega$,
    ylabel={$1/\xi_z$},
    xmin=0, xmax=\textwidth,
    ymin=0, ymax=\textwidth,
    xtick={0,1,2,3},
    ytick={0,1,2,3},
]
\addplot[mark=*,mark size=3pt] coordinates{(0,0) (1,1) (2,2) (3,3)};
\addplot[mark=x,mark size=3pt] coordinates{(0,0) (1,1) (2,2) (3,3)};
\end{axis}
\end{tikzpicture}
\begin{tikzpicture}
\begin{axis}[
    title={$\tilde{\chi}_\perp(\omega)$},
    xlabel=$\omega$,
    ylabel={$1/\xi_\perp$},
    xmin=0, xmax=\textwidth,
    ymin=0, ymax=\textwidth,
    xtick={0,1,2,3},
    ytick={0,1,2,3},
]
\addplot[mark=*,mark size=3pt] coordinates{(0,0) (1,1) (2,2) (3,3)};
\addplot[mark=x,mark size=3pt] coordinates{(0,0) (1,1) (2,2) (3,3)};
\end{axis}
\end{tikzpicture}
\caption{The longitudinal (left) and transverse (right) dynamic susceptibility of the pseudo spin at the impurity site in $d = 2$. The longitudinal susceptibility starts with $\omega^3$ at low-frequencies and behaves as $\omega^{1-2/\nu_z}$ at large frequencies. On the other hand, the transverse susceptibility diverges as $1/\omega^\eta$ at low frequencies and decays as $1/\omega^{2/\nu_\perp - 1}$ at large frequencies. The crossover for the susceptibilities occurs at the inverse correlation length $\omega \sim 1/\xi_{z,\perp}$, respectively.}
\end{figure}

It is also interesting to compare the dynamics of the $XY$ Bose Kondo model to that of the $SU(2)$ Bose Kondo model [70, 71]. The latter can be found in a two-dimensional $O(N \geq 3)$ quantum critical environment such as the paramagnetic-antiferromagnetic quantum critical point. When the $SU(2)$ spin-rotational symmetry exists, the transverse and longitudinal dynamic susceptibilities are controlled by the same exponent $\nu_z = \nu_\perp = \nu$. The low-frequency part of the susceptibilities is then expected to diverge as $1/\omega^\eta$ when $\omega \to 0$, and the high-frequency part decays as $1/\omega^{2/\nu - 1}$ as $\omega \to +\infty$, where the exponent satisfies the inequality $\nu < 2$ because the impurity can not fluctuate faster than the environment. As a result, in
the $SU(2)$ Bose Kondo model, not only the transverse dynamic susceptibility but also the longitudinal one behaves as in Fig. 6.2 (right). From this comparison, we learn that the behavior of the longitudinal dynamic susceptibility shown in Fig. 6.2 (left) is a rather unique property of the $XY$ Bose Kondo model.

### 6.3.2 Halon Density Profile

The charge density profile of the halon. The charge is separated into a non-universal part and an universal part. The non-universal part is localized at a microscopic scale $r_{uv}$. The universal part carries the charge $\pm 1/2$, which is distributed up to a critically large length scale $r_0$. At $r \gg r_0$, the density profile acquires a linear-response shape.

**Figure 6.3.** The charge density profile of the halon. The charge is separated into a non-universal part and an universal part. The non-universal part is localized at a microscopic scale $r_{uv}$. The universal part carries the charge $\pm 1/2$, which is distributed up to a critically large length scale $r_0$. At $r \gg r_0$, the density profile acquires a linear-response shape.

In this subsection, we discuss the density profile of the halon. For simplicity, we only consider the most experimentally relevant trajectory ($h_z \to 0, h_\perp = 0$). In this case, the only macroscopic characteristic length scale of the system is $\xi_z$. The physical meaning of this length scale in the spatial directions is the healing length,

$$r_0 \equiv \xi_z \sim |h_z|^{-\tilde{\nu}_z}. \quad \text{(6.37)}$$
At $r \ll r_0$, the bosonic field is strongly influenced by the impurity and the correlation functions are controlled by the boundary quantum criticality; while at $r \gg r_0$, the impurity degrees of freedom get screened and the correlation functions of the bosonic field restore their bulk quantum critical behavior. In the halon case, $r_0$ naturally gives the radius of the halo.

Using the standard thermodynamic relation for the averaged partial derivative of the Hamiltonian, we find the following result for the singular part of the $z$-projection of the impurity spin (negative/positive sign corresponds to positive/negative $h_z$):

\[
\langle S_z \rangle = \frac{\partial F_s}{\partial h_z} \propto \mp |h_z|^{\nu_z-1} \propto \mp r_0^{1-1/\nu_z}.
\] (6.38)

where $F_s$ is the singular part of the free energy given by Eq. (6.24). A crucial difference between Eqs. (6.38) and (6.24) is that the critical contribution to the energy comes from the distances $\sim r_0$, while the $z$-projection of the impurity spin is an essentially local quantity. The latter circumstance is quite important: It implies that Eq. (6.38) is representative of the scaling of the singular part of any generic local observable.

In view of the divergent radius $r_0$ and scale invariance of the long-wave properties of the critical environment, the structure of the halo has to be described by a scaling function $f$ shared by all the systems within a given universality class of the boundary quantum phase transition:

\[
\delta n(r) = \pm r_0^{-d} f(r/r_0) \quad (r \gg r_{uv}).
\] (6.39)

Here $r_{uv} \ll r_0$ is a system-specific ultraviolet cutoff.

The generic scaling for local observables, Eq. (6.38), implies the following structure of the halo at $r \ll r_0$:

\[
f(x) \propto \frac{1}{x^s} \quad (x \ll 1),
\] (6.40)

\[
s = d - 1 + 1/\tilde{\nu}_z.
\] (6.41)
To arrive at (6.40)–(6.41), observe that by continuity, the relation (6.39) remains meaningful—at the level of order-of-magnitude estimates—down to \( r = r_{uv} \), where we have \( \delta n(r_{uv}) \sim |h_z|^{\nu_{E}-1} \sim r_0^{z-1/\nu_z} \). It is also useful to write the law (6.40)–(6.41) in the form

\[
\delta n(r) \propto \frac{1}{r_0^{d-s} r^{s}} \quad (r_{uv} \ll r \ll r_0).
\]

(6.42)

Note that the above-mentioned bound \( \tilde{\nu}_z > 1 \), implying \( s < d \), guarantees the following two consistency conditions for the halo: (i) The integral over \( r \) should converge at \( r \to 0 \) and (ii) the amplitude of the singular inner part of the halo should vanish on approach to BQCP.

The shape of the outer part of the halo is dictated by a very simple perturbative physics. At \( r \gg r_0 \), the boundary-critical fluctuations are suppressed leaving no room for non-linear effects. The environment thus demonstrates a generic linear response identical—up to the global amplitude—to the response caused by weak local perturbation

\[
H_{\text{pert}} = \tilde{V}\hat{n}(r = 0).
\]

(6.43)

Hence, at \( r \gg r_0 \), the charge density profile satisfies the Kubo formula

\[
\delta n(r) \propto \int d\tau \langle [\hat{n}(r, \tau) - \bar{n}] [\hat{n}(0, 0) - \bar{n}] \rangle.
\]

(6.44)

Although in a quantum-critical environment, the particle number, which is a Noether charge, does not have anomalous scaling dimension and its density has a scaling dimension \( d \). Actually, since the bulk system features the Lorentz symmetry, the space-time density-density correlator in the r.h.s. of (6.44) is expected to demonstrate a power-law behavior: \( \sim 1/(r^2+\tau^2)^d \).

We thus have

\[
f(x) \propto \frac{1}{x^\alpha}, \quad \alpha = 2d - 1 \quad (x \gg 1),
\]

(6.45)
or, equivalently,

$$\delta n(r) \propto \frac{r_0^{\alpha-d}}{r^\alpha} \quad (r \gg r_0). \quad (6.46)$$

As we discussed in Sec. 5.3, the vanishing compressibility is a necessary condition for charge quantization. In terms of the correlator (6.44), that means $\alpha > d$ or $d > 1$. The very same condition follows from the requirement that the integral of $\delta n(r)$ over $r$ be convergent at $r \to \infty$. Then, according to (6.46), the condition $\alpha > d$ implies the divergence of the amplitude of the linear-response tail on approach to BQCP.

### 6.3.3 The Global Compressibility

A system at a quantum critical point is rather fragile so that one halon can change some macroscopic response functions like the total compressibility. This quantity controls the response of the system to a small uniform static potential $\delta U$,

$$\hat{H}[\delta U] = \hat{H} - \hat{N}\delta U, \quad (6.47)$$

where $N$ is the total particle number deviation. Since the total particle number is a conserved quantity, the scaling dimension of operator $\hat{N}$ cannot renormalize. As a result, the field $\delta U$ has the same scaling dimension as the temperature. This implies the scaling ansatz of the total compressibility,

$$\kappa_{\text{tot}} \equiv \frac{\partial^2 F_s}{\partial \delta U^2} = \frac{1}{T} C(h_z T^{-1/\nu_z}), \quad (6.48)$$

where the hyperscaling hypothesis, Eq. (6.24), for the singular part of the total free energy is used. For simplicity, we only consider the $h_z$ field. Since the temperature in experiments is finite, we take the temperature $T = 1/\beta$ as the inverse characteristic length scale. In some experimental systems, like ultracold atoms in optical lattices, the system sizes $L$ can be comparable to the correlation length. Then the universal function $C(x)$ also depends on the space-time ratio $\beta/L$. We also point out that the total compressibility contains no
analytic contributions. This follows from the observation [17] that a small detuning from the bulk QCP can drive the system into an insulator phase, which is incompressible.

At the BQCP, the total compressibility $C(0)/T$ contains contribution from both the impurity and the environment. When tuning away from the BQCP, the total compressibility saturates to $C(\infty)/T$. In this limit, the impurity degree of freedom is frozen, so that the universal constant $C(\infty)$ is the same as the total compressibility of a bulk quantum critical system without the impurity. It is then natural to define the impurity compressibility at the BQCP as the difference,

$$\kappa_{\text{imp}} = \frac{C(0) - C(\infty)}{T}. \quad (6.49)$$

If the system size is finite, the difference $C(0) - C(\infty)$ also depends on the space-time ratio $\beta/L$. Indeed, for $\beta/L = 0$, which is the thermodynamic limit, Ref. [73] calculates the impurity compressibility in an $O(2)$ quantum critical environment to be roughly 0.734; while for the ratio $\beta/L = 1$, our Monte Carlo simulations determine the impurity compressibility to be 0.264(3) (see Sec. 6.5). For other space-time ratios in the range $(0, 1)$, a number in between is expected for the impurity compressibility.

In the spin language, the impurity compressibility $\kappa_{\text{imp}}$ should be regarded as the effective impurity spin susceptibility. Since this quantity has a Curie-like divergence at low temperatures, similar to the $SU(2)$ Bose Kondo problem in the Ref. [70], one can define an effective spin $S^*$ for the impurity. The universal value of $S^*$ does not depend on the microscopic physics and can be derived from $S^*(S^* + 1)/3 = C(0) - C(\infty)$. In general, it is neither an integer nor a half-odd integer.

It is also inspiring to compare the quantity $\kappa_{\text{imp}}$ at the BQCP to other boundary phase transition points. For the transition point of the type of Fig. 5.2 (a), the spin impurity is effectively decoupled from the environment, and we expect the physics of a free spin

$$\kappa_{\text{imp}} = S(S + 1)/3T = 1/4T \quad (\text{with } S = 1/2).$$

On the other hand, if the spin impurity is
entirely screened by the environment, as in Fig. 5.2 (c), the impurity degree of freedom is no longer visible in a global response function, so that the impurity contribution \( \kappa_{\text{imp}} \) will be zero. Hence, measuring the total compressibility allows us to distinguish those three scenarios in experiments.

### 6.4 Numerical simulations of quantum models

In this section, we reveal the halon physics in the superfluid–Mott-insulator quantum critical environment (realized in the Bose Hubbard model) and the paramagnet-antiferromagnet quantum critical environment (realized in the dimmerized quantum Heisenberg model). We perform worm-algorithm quantum Monte Carlo simulations and find that both systems feature boundary quantum critical points.

#### 6.4.1 Bose Hubbard model

We first study the halon physics in the superfluid–Mott-insulator quantum critical environment.

To extract an accurate value of the universal critical exponent \( \tilde{\nu} \), as well as to validate relation (6.40), we simulate not only the standard Bose-Hubbard model (6.1) on the square lattice [17] with the trapping center located at the site \( i = 0 \), but also the 3D classical J-current model:

\[
H = \frac{1}{2K} \sum_{i, \hat{\epsilon} = \hat{x}, \hat{y}, \hat{\tau}} J_{i, i+\hat{\epsilon}}^2 - V \sum_{\hat{\imath} = (0, \tau)} J_{i_0, i_0 + \hat{\imath}}.
\]  

(6.50)

Here \( J_{i, i+\hat{\epsilon}} \) are integer-valued bond currents between neighboring sites. The currents are subject to the zero-divergency constraint: For each site, the algebraic sum (incoming minus outgoing) of all the currents has to be zero. As before, \( V \) is the strength of the center potential. The latter acts only on \( J_{i_0, i_0 + \hat{\tau}} \) (i.e., along the imaginary-time direction at the...
origin). We work with the minimalistic model in which the currents $J_{i,i+\hat{e}}$ take only three values: $\{-1,0,+1\}$. The U(1)-type phase transition occurs at $K_c = 0.333205(2)$.

Without loss of generality, we consider the repulsive case, $V > 0$, so that the two competing ground states of the center have the charges $q_1 = 0$ and $q_2 = -1$ (the charge number $q$ has the physical meaning of the particle number deviation in the Bose Hubbard model and imaginary-time-directed current number deviation in the J-current model). Our main observable is the integral (sum) of the density deviation profile up to a certain distance $r$ from the center ($r_i$ is the distance of the site $i$ from the center):

$$ I(r) = \sum_{r_i \leq r} (n_i - 1). \tag{6.51} $$

For a system of the size $L \times L$, the distance $r$ is in the range $[0, L/\sqrt{2}]$. The charge of the center is defined in the thermodynamic limit:

$$ q = I(\infty). \tag{6.52} $$

In view of the above-mentioned asymptotic behavior $\delta n \propto 1/r^3$, the saturation of $I(r)$ to $q$ is rather slow:

$$ I(r) = q \pm \frac{\text{const}}{r} \quad (r \to \infty). \tag{6.53} $$

For a compelling demonstration of quantization of $q$ it is thus very desirable to find an appropriate way of dealing with finite-size corrections. To this end we observe that for the system size $L \gg r_0$, equation (6.53) implies the following scaling ansatz:

$$ I(r) - q = \pm L^{-1} f(r/L) \quad (r_0 \ll r \ll L), \tag{6.54} $$

where $f(x)$ is a certain scaling function such that $f(x) \propto 1/x$ at $x \ll 1$. An accurate calculation of $q$ amounts then to checking the consistency of ansatz (6.54).
Apart from the finite-size effects there are also finite-temperature corrections. In our simulations, the temperature is adjusted to the system size by

\[ T = \frac{c}{L}, \]

(6.55)

where \( c \) is the sound velocity, which is 4.8(2) for Bose Hubbard model [2] (for J-current model, \( c = 1 \) in view of explicit symmetry between all the three directions). This choice is natural in view of the space-(imaginary-)time symmetry of U(1) criticality. The finite-temperature effects then reduce to a certain quantitative change of the form of the function \( f(x) \) at \( x \sim 1 \), which does not alter the numeric protocol.

Figure 6.4. The integral \( I(r) \) at \( V = 3.5 \) and different system sizes \( L \). The simulation is performed in the canonical ensemble with the total number of particles \( N = L^2 \). The inset shows consistency with the scaling ansatz (6.54) with \( q = 0 \), thus simultaneously verifying the linear-response asymptotic behavior (6.53) and the fact that the center charge equals zero. In this and other plots, the error bars do not exceed symbol sizes. The apparent noise—vanishing in the long-range limit—is totally due to the discreteness of the system.
In Fig. 6.4 we present the results for the case $V = 3.5$. This value of $V$ is twice smaller than $V_c = 6.86(8)$ (established below) and large enough for non-linear response to take place at short distances. Consistency with the ansatz (6.54) confirms the linear-response asymptotic behavior (6.53) and demonstrates that $q = 0$ within our numeric resolution.

To accurately resolve universal features of the criticality of the transition between the $q = 0$ and $q = -1$ states, we resort to the J-current model in a (pseudo) grand canonical ensemble; see Fig. 6.5. In optical lattice emulators, similar analysis can be performed if the role of particle reservoir is played by the peripheral region of the system. In this case, the total number of particles is not a relevant observable any longer. A way out is to deal with $I(r)$ at a certain large $r$. To model such setup with the Hamiltonian (6.1), we take $r = L/2\sqrt{2}$ corresponding to one half of the largest possible $r$. The data presented in Fig. 6.6 is consistent with what we have learned from J-current model.

A remark is in order here concerning the unambiguity of our conclusion about the nature of the transition. The temperature scaling (6.55) creates a potential concern that the $L$-dependence of the data might be merely a reflection of finite-temperature smearing of the “first-order” transition between two distinct ($q = 0$ and $q = -1$) ground states coexisting at $V = V_c$. What excludes this scenario in our case is the value of $\tilde{\nu}$. Indeed, the “first-order” scenario would mimic $\tilde{\nu} = 1$, because the energy difference between two competing states would be directly proportional to $V - V_c$, so that the characteristic range of the finite-temperature smearing would be $|V - V_c| \sim T \sim 1/L$.

In Fig. 6.7, we numerically validate the result (6.40) for the inner part of the halo. Integration of Eq. (6.40) over $r$ leads to the scaling ansatz $I(r) = q_{core} \pm C_0 (r/r_0)^{2-s}$, where $q_{core}$ is the charge of the core and $C_0$ is a dimensionless constant. (The value of $C_0$ depends on the free order-unity prefactor in the definition of $r_0$; in particular, the definition can be fixed by requiring that $C_0 = 1$.) In the canonical ensemble, similar ansatz, up to replacing $r_0 \to L, C_0 \to C_1$, applies to a system of a finite size at the critical point. Qualitatively, this
Figure 6.5. The change in the total number of particles, $\Delta N$, in the J-current model as a function of rescaled strength of the center at different system sizes $L$. The simulation is performed in the pseudo-grand-canonical ensemble containing only the two (most relevant) sectors of the total particle number: $N = L^2$ and $N = L^2 - 1$. Optimal fitting yields $V_c = 1.5056(5)$ and $\nu = 2.33(5)$. The inset shows bare (not scaled) data.

case corresponds to $r_0 \sim L$, all the quantitative difference being captured by the value of the constant $C_1$ (sensitive, in particular, to the boundary condition and the finite temperature $T \gtrsim 1/L$). The data in Fig. 6.7 demonstrate consistency with this scaling ansatz, with $C_1$ indistinguishable from $1/2$ within our numeric resolution.

6.4.2 Dimmerized Heisenberg model

While the halon physics is in the two-dimensional $O(N)$ quantum rotor models for $N > 1$, we have not related them to the real-world quantum models except the case of $N = 2$. In this section, we introduce an experimentally relevant implementation of the $O(N = 3)$ halon in a dimmerized Heisenberg antiferromagnet.
Figure 6.6. The integral $I(L/2\sqrt{2})$ in the Hubbard model as a function of rescaled strength of the center at different system sizes. The simulation is performed in the grand canonical ensemble. The data are consistent with the scaling analysis of the transition in J-current model (see Fig. 6.5). The value $V_c = 6.86(8)$ is obtained from optimal fitting with $\tilde{\nu} = 2.33(5)$.

The environment we discuss is a square lattice spin model with two different coupling strengths,

$$\hat{H}_{AF} = J \sum_{\langle i,j \rangle} \hat{S}_i \cdot \hat{S}_j + J' \sum_{\langle i,j' \rangle} \hat{S}_i \cdot \hat{S}_j,$$

(6.56)

where $\hat{S}_i$ are spin-$1/2$ operators on lattice sites, and the exchange coupling between different sites form a coupled-dimmer pattern as shown in Fig. 6.8. The dimensionless coupling $J'/J$ controls the zero temperature phase diagram of the system. When the inner-dimmer coupling $J'$ dominates the system, the ground state is a paramagnet consisting of an array of singlets. On the other hand, when the inter-dimmer coupling $J$ dominates, the ground state is an antiferromagnet where neighboring spins point in the opposite directions. A continuous
Figure 6.7. Revealing the singularity of the inner part of the halo with the J-current model simulated at the critical point in the canonical ensemble \( N = L^2 \). The dashed lines are only to guide the eye. In the macroscopic limit and at \( r/L \ll 1 \), the curves saturate to the law \( I(r) + 1/2 = C_1(r/L)^{2-s} \). The solid line represents this law with \( s = 1.43 \) and \( C_1 = 1/2 \).

Quantum phase transition happens at \( J'/J = 1.9096(2) \)[76], and the infrared physics of this critical point is described by a \((2 + 1)\)-dimensional \( O(3) \) critical theory.

This model has wide applications in condensed matter physics. It describes dimmerized antiferromagnetic materials like \( \text{TlCuCl}_3 \). It is also relevant to the effective physics of many exotic electron systems, such as the \( \text{CuO}_2 \) layers of the cuprate superconductors [77] and double-layered integer quantum Hall systems[78]. In the near future, we expect that such lattice spin systems can be realized in ultracold fermions in a two-dimensional optical double-well superlattice potential [79, 80, 81].

The long-wave-length properties of the dimmerized antiferromagnet is captured by the \( O(3) \) quantum rotor model (6.10). A rotor is defined for each unit cell and can be considered as an effective representation of a pair of antiferromagnetically coupled spins. The rotor
Figure 6.8. A composite local-magnetic-field impurity in a dimmerized Heisenberg antiferromagnet. The environment is a spin system on a coupled-dimer lattice. The exchange couplings are $J'$ for the solid red bonds and $J$ for the blue bonds. The impurity is a local magnetic field coupled to the spin-z projection of a pair of spins in the same unit cell.

orientation operator $\hat{\mathbf{n}}_i$ corresponds to the local staggered magnetization $\hat{\mathbf{S}}_i - \hat{\mathbf{S}}_j$ where $i, j$ are sites in the same unit cell. The rotor angular momentum operator $\hat{\mathbf{L}}_i$, which plays the role of the Noether charge density, corresponds to the local uniform magnetization in each unit cell $\hat{\mathbf{S}}_i + \hat{\mathbf{S}}_j$.

In the quantum rotor model, a local-field impurity coupled to the angular momentum operator as Eq. (6.13) gives rise to a halon near the BQCP. We expect the same physics to emerge for the following impurity Hamiltonian in the dimmerized antiferromagnet environment,

$$\hat{H}_{\text{imp}} = V[\hat{S}_z(r_0) + \hat{S}_z(r_0 + \hat{e}_x)],$$

where the impurity is a local magnetic field $V$ coupled to two spins in the same unit cell. When the field strength $V$ increases to a BQCP $V_c$, the singlet state in the unit cell eventually
breaks down to a direct product state, causing the total charge \( Q \) to abruptly change by one spin-projection quantum.

To test the above theoretical predictions, we employ large-scale quantum Monte Carlo simulations for the impurity Hamiltonian (6.56) and (6.57). In Fig. 6.9, we show the total charge \( Q \) as a function of the local field strength \( V \). Our data clearly suggest a BQCP at \( V_c/J = 2.40(2) \). The boundary critical exponent associated with the halo size is calculated to be \( \tilde{\nu}_z = 2.32(8) \). Just as the \( O(2) \) counterpart, this exponent is also larger than 2. Correspondingly, the linear response dynamics discussed in Sec. 6.3 also applies to the \( O(3) \) halon.

![Figure 6.9](image-url)

**Figure 6.9.** The total uniform magnetization in the dimmerized Heisenberg model as a function of the rescaled strength of the local field at different system sizes. The simulation is performed in the grand-canonical ensemble. The boundary quantum critical point is determined at \( V_c/J = 2.40(2) \) and a boundary critical exponent for the halo size is calculated to be \( \tilde{\nu}_z = 2.32(8) \).
We emphasize that the halon physics is expected only if the local magnetic field is coupled to at least two spins in the same unit cell. Indeed, one can show that there will be no boundary phase transition at all if the local field is coupled to only one spin,

$$\hat{H}_{\text{imp}} = V\hat{S}_z(\mathbf{r}_0).$$  

(6.58)

Since the spin at the site $\mathbf{r}_0$ is paired with another spin in the same unit cell, the local spin polarization at the site $\mathbf{r}_0$ will be compensated by the paired spin. As a result, the total charge $Q$ of the system will remain to be zero no matter how strong the local field strength is, leaving no room for the halon physics to develop.

Although the above discussion is sufficient to demonstrate that the $O(3)$ halon physics is experimentally relevant, we want to briefly discuss the Bose Kondo impurity counterpart of Eq. (6.57). This impurity model is probably less relevant to experiments, but provides an interesting theoretical implementation of the Bose Kondo model on its own. The key observation is that by fine-tuning to the BQCP, the degeneracy between the singlet/direct-product states can be effectively described by a pseudo-spin-1/2 degree of freedom. The Bose Kondo model is then introduced by replacing two physical spins in the same unit cell with one pseudo-1/2-spin, and coupling the pseudo-spin to the neighboring physical spins via an XY-type interaction,

$$\hat{H}_{AF} \rightarrow \hat{H}_{AF} + \gamma \sum_n \left[ \hat{S}_+ \hat{S}_-(\mathbf{r}_n) + \hat{S}_- \hat{S}_+(\mathbf{r}_n) \right] + h_z \hat{S}_z,$$  

(6.59)

where the sum of sites $\mathbf{r}_n$ goes over all nearest neighbors of the unit cell, which is now replaced with the pseudo-impurity. One advantage of working with this model is that the BQCP is exactly known to be $h_z = 0$ by the explicit spin-flip symmetry.
6.5 Numerical simulations of effective models

In this section, we perform a comprehensive worm-algorithm study of the universal properties of the halon in an $O(2)$ quantum critical environment. As long as we are only interested in the critical properties, we are allowed to maximally simplify the model to gain an increase in efficiency. This can be achieved by i) working with the improved $J$-current model which almost eliminates the bulk finite-size corrections and ii) simulating the Bose Kondo model instead of the static impurity model so that the symmetry of the BQCP is implemented at the microscopic level. We confirm that the Bose Kondo model (6.15) captures the universal critical physics of the static impurity model (6.13). We also extract the values of the critical exponents and various universal constants for the halon boundary phase transition.

6.5.1 Modified $J$-current model

The simplest model for simulating the $O(2)$ criticality is the (fully classical) $J$-current model [21]. In the $d = 2 + 1 = 3$ case, the model consists of integer currents $J$ living on the bonds of a three dimensional $L^2 \times L_\tau$ cubic lattice, with $L$ as the size of the spatial dimensions and $L_\tau$ as the size along the “temporal” direction (in the absence of the impurity, all the three dimensions are absolutely equivalent). The currents are subject to the zero-divergence constraint,

$$\text{div} \ J = 0,$$  \hspace{1cm} (6.60)

meaning that at each site, the algebraic—incoming minus outgoing—sum of all the currents is zero. To have a really minimalistic model, one also confines the allowed values of the bond currents to just three numbers:

$$J = 0, \pm 1.$$ \hspace{1cm} (6.61)

The Hamiltonian of the model reads
Here the vector \( i = (x, y, \tau) \) labels the sites on the cubic lattice by three discrete coordinates: \( x, y, \) and \( z; \hat{x}, \hat{y}, \) and \( \hat{\tau} \) are the lattice unit translation vectors in corresponding directions; \( J_{i,\hat{e}} \equiv -J_{i+\hat{e},-\hat{e}} \) is the J-current of the bond going from the site \( i \) in the direction \( \hat{e} \).

In terms of the mapping onto a two-dimensional system of lattice bosons (at an integer filling factor), the closed loops of currents should be understood as the worldlines of O(2) charge quanta, with \( J_{i= (x,y,\tau),\hat{\tau}} \) having the meaning of the particle/hole charge on the site \( (x,y) \) at the imaginary-time moment \( \tau \). The zero-divergency constraint guarantees the “conservation of charge”: The quantity

\[
Q = \sum_{x,y} J_{(x,y,\tau),\hat{\tau}}
\]

is the same for any \( \tau \). This way the model (6.60)–(6.62) describes the universal properties of the insulator-to-superfluid criticality; the corresponding transition takes place at the critical value \( K_c = 0.3332052(20) \) [10] of the control parameter \( K \).

Although we can simulate systems with size as large as \( L = 512 \), many universal observables still suffer from significant non-universal finite-size corrections. To suppress those corrections, we find that it is very useful to introduce an improved J-current model by making the coupling strength \( K \) in Eq. (6.62) to be current-dependent,

\[
H'_J = \sum_{i,\hat{e}} \frac{1}{2K(J_{i,\hat{e}})} J_{i,\hat{e}}^2 \quad (\hat{e} = \hat{x}, \hat{y}, \hat{\tau}).
\]

The coupling \( K(J) \) needs to be fine-tuned so that the finite size corrections at the critical point are minimized. In the case when there are five allowed values for the currents \((0, \pm 1, \pm 2)\), we find the optimized coupling strengths to be \( K(0) = K(\pm 1) = 0.32944986(10) \)
and $K(\pm 2) = 0.16891892$ at the space-time ratio $L_{\tau}/L = 1$. In what follows, by default, we present the results for the minimal J-current model (6.62). However, for some quantities with bad finite size corrections, we will employ the improved J-current model (6.64).

We now discuss the impurity problem in the J-current models. A static spinless impurity (call it a center to avoid confusion with the spin-1/2 impurity) is introduced by the following term

$$H_{\text{center}} = V \sum_{\tau} J_{(0,0,\tau),\hat{\tau}},$$

with $V$ controlling the strength of the impurity [in view of the particle-hole symmetry of the model (6.60)–(6.62), the sign of the impurity plays no role]. We studied the model (6.62) with (6.65) in our previous work [13], where we found that the halon BQCP is $V_c = 1.5056(5)$, and the value of the exponent is $\tilde{\nu} = 2.33(5)$.

Here we must admit that the model (6.60)–(6.65) is not yet optimal. Indeed, adding the term (6.65) to the model (6.60)–(6.64) breaks the particle-hole symmetry of the latter, so that one has to fine-tune the parameter $V$ to the unknown a priori critical $V_c$. A more efficient approach is to introduce a spin-1/2 impurity thus preserving the particle-hole symmetry at zero magnetic field, analogously to how it is done for the quantum rotor model, see Eq. (6.15). This amounts to requiring that on the bonds going from the sites $(0,0,\tau)$ in the direction $\hat{\tau}$, there lives a half-integer current

$$S_{\tau} = \pm 1/2.$$  

(6.66)

For the sites involving the half-integer currents $S$, the zero-divergency condition also includes the algebraic sum of the two half-currents associated with this site, which guarantees the conservation of charge: the $\tau$-independence of the quantity $Q$, where

$$Q = S_{\tau} + \sum_{x,y} J_{(x,y,\tau),\hat{\tau}}.$$  

(6.67)

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Following the principle of minimalism, we also restrict the values of the J-currents on those bonds to zero:
\[ J_{(0,0,\tau),^x} = 0. \]  \hspace{1cm} (6.68)

One should not confuse this constraint with decoupling the spin-1/2 impurity from the J-current environment. The coupling is still there due to the currents \( J_{(0,0,\tau),^x} \) and \( J_{(0,0,\tau),^y} \); see Fig. 6.10 for an illustration. [In terms of the analogy (a slight contrast) to the quantum rotor model (6.15), our spin-1/2 impurity interacts with the nearest-neighboring rotors, which allows us to apply the constraint (6.68) thus safely removing the rotor on the impurity site.]

![Illustrative configuration of the bond currents](image)

**Figure 6.10.** Illustrative configuration of the bond currents for the J-current model with a spin-1/2 impurity at the origin in \((1 + 1)\) dimension. The impurity half-currents \( S_{\tau} \) are shown with arrows. The impurity couples to the environment via the bond currents in the spatial direction.

To complete the minimalistic model, we just need to introduce the coupling between the half-currents and the magnetic field:
\[ H_{\text{spin}} = h_z \sum_{\tau} S_{\tau}. \]  

It is, however, important to mention that the finite-size effects prove to be rather sensitive to the strength of the coupling of the impurity to the environment. To control those effects, we change the weights of the currents \( J_{(0,0,\tau),\hat{x}} \) and \( J_{(0,0,\tau),\hat{y}} \) in the Hamiltonian (6.62):

\[
\frac{1}{2K} J_{(0,0,\tau),\hat{e}}^2 \rightarrow \frac{1}{2K_I} J_{(0,0,\tau),\hat{e}}^2 \quad (\hat{e} = \hat{x}, \hat{y}),
\]

so that while the value of \( K \) is fixed at \( K_c \), the value of \( K_I \) is a free parameter, which can be optimized to improve the efficiency of the scheme.

### 6.5.2 Global Response Functions

Consider the universal compressibility when approaching the BQCP along the trajectory \((h_z \rightarrow 0, h_x = 0)\).

In our simulations, we set the space-time ratio to be unity \((L_\tau/L = 1)\) for convenience, so that the scaling ansatz Eq. (6.48) for the total compressibility predicts \( \kappa_{\text{tot}}/L \sim C(h_z L^{1/\nu_z}) \), where \( C(x) \) is a universal function.

We analyze the universal function \( C(x) \) at \( x = 0 \) (i.e., at the critical point \( h_z = 0 \)) first. In Fig. 6.11, we present the finite size scaling flows for the rescaled compressibility at the BQCP, which is expected to saturate to a universal constant \( C(0) \) in the thermodynamic limit. We compare the flows for models with different impurity-environment interaction \( K_I \). For all the models, the flows extrapolate to the same universal constant \( C(0) = 0.780(3) \). This suggests that they share the same universal theory in the long-wavelength limit. Furthermore, the opposite trends for the models with \( K_I < 0.6 \) and \( K_I > 1.0 \) indicate that this universal theory has an intermediate effective coupling strength \( 0.6 < K_I^* < 1.0 \). Unfortunately, the exact value of \( K_I^* \) is hard to determine accurately because the models suffer from non-monotonic finite-size corrections.
For comparison, we also calculate the flow of the static impurity model (6.65). Interestingly, the flow is almost identical to that of the spin impurity model with a coupling strength $K_I = K_c$, where $K_c$ is the bulk critical coupling strength in Eq. (6.62). This observation indicates that the spin impurity model is an excellent approximation to the original static impurity model.

**Figure 6.11.** The finite size scaling flows of the rescaled charge compressibility at the boundary critical point. The spin impurity models with different coupling strength $K_I$, as well as the static spinless impurity model, are compared. All flows tend to converge to the same universal value, which is extracted to be $C(0) = 0.780(3)$.

We now discuss the universal compressibility as a function of the detuning $h_z$. We find that the impurity model defined in the original J-current model (6.62) is not useful in this case due to a strong finite-size corrections. We therefore employ the improved J-current model (6.64) with an optimized coupling strength $K_I = 0.43$. We use this model to calculate the compressibility curves for different system sizes. After rescaling the magnetic field $h_z \rightarrow h_z L^{1/\nu_z}$, we find that all curves—even for relatively small system sizes—collapse nicely by
setting the boundary critical exponent to be $\tilde{\nu}_z = 2.33$, which is the same as the exponent of the halo size in Eq. (6.37). The master curve, which is the universal compressibility $C(x)$, contains rich physics. The universal value at the BQCP is found to be compatible with the universal value $C(0) = 0.780(3)$ obtained from the original J-current model 6.62. This implies that both models have the same universal physics. We also notice that $C(x)$ eventually saturates to a constant $C(\infty)$ at large $h_z$ and low temperature. The value of $C(\infty)$ is consistent with the universal constant 0.5160(6), which is the total compressibility calculated for the bulk quantum critical system when the impurity is absent[10]. We find the effective impurity spin susceptibility at the BQCP to be $[C(0) - C(\infty)]/T = 0.264(3)/T$. Despite the fact that the spin impurity is strongly coupled to the environment, the effective spin susceptibility is only slightly different from that of an isolated spin impurity, which is $S(S + 1)/3T = 1/4T$ (with $S = 1/2$).

6.5.3 Impurity Dynamics

Having described the system’s response to a global field, we turn to the discussion of the spin impurity’s response to a local magnetic field, namely $h_z$ and $h_x$. These responses can be characterized by two spin correlation functions $\chi_{z,\perp}(\tau) \equiv \langle \delta \hat{S}_{z,\perp}(\tau)\delta \hat{S}_{z,\perp}(0) \rangle$, where $\tau$ is the imaginary-time variable. Their scaling ansatz is given by Eq. (6.26).

Right at the BQCP, the long-time correlations decay following the power-law with a boundary critical exponent. In Fig. 6.13, it is clearly seen that the transverse correlation function develops a power-law tail. We expect that the tail decays as $1/\tau^{2-2/\tilde{\nu}_\perp}$ and that it dominates the static transverse susceptibility, so that $\chi_{\perp}(i\omega = 0) \sim L^{2/\tilde{\nu}_\perp-2}$. By fitting the numerical data for the static transverse susceptibility, we determine the boundary critical exponent $\tilde{\nu}_\perp = 1.15(3)$.

In Fig. 6.14, we show the longitudinal correlation function at the BQCP, which also develops a power-law behavior at a large time scale. This tail is consistent with the power-
law decay with the exponent $2 - \frac{2}{\tilde{\nu}_z}$, with $\tilde{\nu}_z = 2.33(5)$ the exponent for the halo size in Eq. (6.37). Unfortunately, we are not able to extract the exponent $\tilde{\nu}_z$ directly from the longitudinal static susceptibility $\chi_z(i\omega = 0)$. This is because the universal tail contribution to the static susceptibility $\chi_z(i\omega = 0) \sim L^{2/\tilde{\nu}_z-2}$ is subleading due to a large exponent $\tilde{\nu}_z > 2$.

Once moving away from the BQCP with a small but finite magnetic field $h_z$, a macroscopic correlation time $\xi_z \sim |h_z|^{-\tilde{\nu}_z}$ emerges. By the scaling ansatz (6.26), we expect that the universal correlation function $\Psi_z(x)$ is controlled by different physics at the short- and long-time limits. The short-time behavior within the correlation time coincides with the universal correlation function right at the BQCP as in Fig. 6.14, while the long-time behavior is expected to decay as $\sim \tau^{-4}$. Due to the relatively large exponent, the long-time physics turns out to be extremely difficult to resolve within a single simulation box. Nevertheless, we
Figure 6.13. The transverse correlation function in the imaginary time direction at the impurity site. The long-time correlation function has a power law decay. The corresponding critical exponent is found to be $2 - 2/\nu_\perp = 0.26(3)$, or $\nu_\perp = 1.15(3)$, which is extracted by fitting the finite size scaling of the xy static susceptibility.

are able to overcome this subtlety and calculate the entire universal longitudinal correlation function $\Psi_z(x)$—see Fig. 6.15—by using the flowgram method[82, 83]. We first calculate various longitudinal correlation functions for different magnetic fields, then rescale $\tau \rightarrow \tau h_z^{\nu_z}$ and $\chi_z(\tau) \rightarrow \chi_z(\tau) h_z^{2\nu_z-1}$ to match the universal parts of different correlation functions. We observe an excellent collapse onto a master curve, which gives the universal function $\Psi_z(x)$ which covers both the short- and long-time scales. From Fig. 6.15, we can clearly see that the universal function starts with $x^{2/\nu_z - 2}$ at small $x$ and eventually decays as $x^{-4}$ at large $x$.

The subtlety of directly observing the long-time tail is clearly seen from this figure. Taking $h_z = 1.0$ as an example, the tail starts to dominate beyond the time scale $\sim 20$. However, the amplitude of the correlation function at this time scale drops to $10^{-6}$, which is already comparable to the typical statistical error in our Monte Carlo simulations.
Figure 6.14. The longitudinal correlation function in the imaginary time direction at the impurity site. The long-time correlation function has a power law decay. The exponent is found to be consistent to $2 - 2/\tilde{\nu}_z$ with $\tilde{\nu}_z = 2.33(5)$.

6.6 Conclusions

We revealed the physics of the halon, which is a special critical state of an impurity in a quantum-critical environment. The hallmark of the halon physics is that a well-defined integer charge gets fractionalized into two parts: a microscopic core with half-integer charge and a critically large halo carrying a complementary charge of $\pm 1/2$. The halon phenomenon emerges when the impurity–environment interaction is fine-tuned to the vicinity of a boundary quantum critical point (BQCP), at which the energies of two quasiparticle states with adjacent integer charges approach each other. The universality class of such BQCP is captured by a model of pseudo-spin-1/2 impurity coupled to the quantum-critical environment, in such a way that the rotational symmetry in the pseudo-spin $xy$-plane is respected, with a small local “magnetic” field along the pseudo-spin $z$-axis playing the role of control parameter driving the system away from the BQCP. On the approach to BQCP, the half-integer
Figure 6.15. Collapse of longitudinal imaginary-time-dependent correlation functions $\chi_z$ for different magnetic fields $h_z$ at the system size $L = 128$. Both axes are properly rescaled so that the universal parts of the correlation functions match each other thus yielding the master curve. This curve starts with a boundary critical behavior $x^2/\tilde{\nu}_z^{-2}$ with $\tilde{\nu}_z = 2.33(5)$ at small $x$ and eventually evolves into asymptotic behavior $x^{-4}$ at large $x$.

projection of the pseudo-spin on its $z$-axis gets delocalized into a halo of critically divergent radius, capturing the essence of the phenomenon of charge fractionalization. With large-scale Monte Carlo simulations, we confirm the existence of halons—and quantify their universal features—in O(2) and O(3) quantum critical systems.
CHAPTER 7
TRAPPING COLLAPSE

The text of this chapter has been adapted from Ref. [14].

7.1 Introduction

Everyone is familiar with the standard quantum mechanical problem of finding bound states in a potential well (“trap”) of radius $R_0$ in one, two, and three dimensions (1D, 2D, and 3D). For simplicity, we assume that the potential is spherically symmetric. While in 3D the trap strength $V$ has to exceed some finite critical value $V_c$ to have one bound state, even an arbitrarily weak trap features a shallow bound state in 1D and 2D; i.e., formally, $V_c = 0$ in low dimensions. For $V - V_c \ll 1/mR_0^2$, with $m$ the particle mass (we will refer to this case as a weak trap), the only bound state $\psi_1$ is extremely “shallow”: the binding energy satisfies the condition $E_1 \ll V - V_c$, and the localization length $l = 1/\sqrt{2mE_1}$ (in the units $\hbar = 1$) is much larger than the well radius $R_0$.

At the single-particle level, the shallow bound state problem is exhaustively treated in textbooks (see, e.g., [84]). However, to the best of our knowledge, the question of how many (strongly) repulsive particles can be localized by a weak trap—and whether the number can be infinite—has been never addressed. One may immediately deal with two simple cases, depending on the particle statistics and dimension of space. (i) A weak trap cannot bind more than one fermion because even in the absence of interactions, the second fermion has to go to the delocalized state with zero energy by the Pauli principle. Thus the best total energy of a pair is $E_2 = -E_1$, and adding repulsive interactions may only increase it
further (as a finite-size effect for a delocalized state). (ii) A dilute repulsive Bose gas in 1D can be mapped onto non-interacting fermions (the so-called Tonks-Girardeau limit) when \( U > 1/2ml^2 = E_1 \), implying that even for relatively weak \( (U \ll V) \) interactions, the trap can bind only one particle, regardless of statistics. [In this work, we focus on short-range repulsive interactions characterized by a typical interaction range \( R_i \sim R_0 \) and potential strength \( U \); its zero-momentum Fourier component will be denoted as \( U(0) \) and the s-wave scattering length, where appropriate, as \( a_s \).]

In all other cases, answering the question requires more elaborate considerations, and, for strong interactions, numerical simulations. The main result of this work is the effect of trapping collapse when in both 2D and 3D cases, weak traps bind infinitely many bosons. When repulsive interactions are relatively weak (the criterion is based on the requirement that adding a particle to the system does not change substantially the structure—and in particular, the density profile—of the state substantially), one can reveal the effect by solving the Gross-Pitaevskii (GP) equation. Remarkably, the phenomenon holds true even when interactions are strong, e.g., for hard-core repulsion between bosons, as our lattice path-integral Monte Carlo (PIMC) simulations confirm. In this case, particles added to the ground state change its structure substantially. Our data in 2D indicate that in this regime, the localization length diverges exponentially with the particle number, and we argue that—despite strong correlations—such a behavior can still be understood based on the GP equation.

### 7.2 The weak interaction limit

The GP approach is justified when many bosons occupy the same mode. For our problem, we reformulate this condition as a requirement that properties of the ground state do not change significantly when adding/removing one particle. More specifically, if a particle is placed into an orbital \( \psi \) with the single-particle binding energy \( E \) and the localization length \( l_E \sim 1/\sqrt{mE} \), the energy of its interaction with the rest of the particles should remain much
smaller than $|E|$. To begin with, this criterion should be satisfied when we add the second particle to the textbook single-particle state $\psi_1$. In 3D, an estimate of the potential energy of repulsion immediately follows from properties of bound $s$-wave states (their asymptotic decay goes as $\psi_1 = 1/r \sqrt{4\pi l}$):

$$U_i \approx \frac{4\pi a_s}{m} \int d^3r |\psi_1(r)|^4 \sim \frac{a_s}{ml^2} \int_{R_0} \frac{dr}{r^2} \sim E_1 \frac{a_s}{R_0}.$$  (7.1)

This leads to the condition for applicability of the GP description of trapped many-particle states

$$a_s \ll R_0 \quad (3D).$$  (7.2)

For short-range interactions with $R_i \sim R_0$, this criterion is no different from the Born approximation condition for inter-particle scattering. Since an integral for potential energy is dominated by distances comparable to the smallest scale in the problem, i.e. the trap radius, this microscopic criterion will not be modified by many-body effects.

Once about $\sim R_0/a_s$ particles are placed on the orbital, the $N$-body state will start evolving towards a more delocalized density profile because the ionization potential defined in terms of a difference between the total $N$-particle energies as $I_N = E_{N-1} - E_N$ will approach zero. To see whether the number of localized particles can be infinite, we solve the static GP equation with zero chemical potential, $\Delta \psi(r) = 8\pi a_s \psi^3$, or

$$\psi''(r) + 2\psi'(r)/r = 8\pi a_s \psi^3.$$  (7.3)

The solution decays at large distances $\psi(r \to \infty) = 1/\sqrt{16\pi a_s \ln(r/R_0)} r$, but this decay is weak: It does not prevent the integral for the total particle number, $N = \int d^3r |\psi(r)|^2 \propto \int dr/\ln(r/R_0)$, from diverging at the upper limit. This establishes the effect of trapping collapse for a weakly interacting 3D system. As for the total interaction energy, the integral $\int d^3r |\psi(r)|^4$ is still dominated by the trap potential region.
Similar considerations apply to the 2D case with one notable exception: the effective repulsive interaction is now scale-dependent with logarithmic renormalization towards smaller value at low energies:

\[ U_{\text{eff}}(k) \approx \frac{U(0)}{1 + g \ln(1/kR_i)}, \quad g = \frac{mU(0)}{2\pi}, \quad (7.4) \]

where \( k \) is the relative momentum of two particles. This formula, in particular, implies that even for strongly repulsive bosons with \( g \gg 1 \), the effective interaction is weak (and universal!): \( mU_{\text{eff}}(k) \to 2\pi/\ln(1/kR_i) \ll 1 \) at low enough energies. An estimate of the potential energy of repulsion for two particles now reads:

\[ U_i \approx U_{\text{eff}}(1/l) \int d^2r |\psi_1(r)|^4 \sim E_1 mU_{\text{eff}}(1/l). \quad (7.5) \]

The integral is dominated by distances of the order \( l \), justifying the use of the effective coupling constant (recall that in 2D the bound state described by the modified Bessel function \( K_0(r/l) \) is only weakly dependent on distance under the localization length). If the interaction is weak, \( mU(0) \ll 1 \), or the state is very shallow, we find that conditions for applying the GP equation to the trapping problem are satisfied. The solution of the radial equation at zero chemical potential,

\[ \psi''(r) + \frac{\psi'}{r} = 2mU_{\text{eff}}(r) \psi^3, \quad (7.6) \]

has the asymptotic form \( \psi(r \to \infty) = \sqrt{\ln(r/R_0)/4\pi/r} \). Here we explicitly consider the universal asymptotic expression for \( mU_{\text{eff}} \). If the value of the constant \( g \) in Eq. (7.4) is small, and the logarithmic flow of the coupling constant can be neglected, then in a broad range of intermediate length scales the solution is simply \( \psi(r) = 1/\sqrt{4\pi g r} \). Again, the integral for the total particle number diverges at the upper limit, \( N \propto \int dr \ln(r/R_0)/r \), indicating that weak traps in 2D can localize infinitely many bosons, including strongly repulsive ones.
Logarithmic dependence of $N$ on the upper cutoff ensures that finite-density corrections to the $U_{\text{eff}}(r)$ dependence on length scale remain sub-leading.

### 7.3 The strong interaction limit

To verify these results, and to explore what happens when conditions for the GP approach are not satisfied in the form of strong inequalities, we resort to PIMC simulations of square/cubic lattice systems with tight-binding dispersion relation $\epsilon(k) = 2t \sum_{\alpha=1}^{d} [1 - \cos(k_\alpha a)]$, where $t$ is the nearest-neighbor hopping matrix element and $a$ is the lattice constant (in what follows, the energy and distance are measured in units of $t$ and $a$, respectively). The trap is introduced as an attractive potential $-V\delta_{r,0}$ placed at the origin. The repulsive pairwise interactions between particles are of the on-site Hubbard form, $U(r_i - r_j) = U\delta_{r_i - r_j,0}$.

In 2D, our study of localized many-particle states was performed for $V = 2$ to ensure that the binding energy is about a factor of one hundred smaller than the bandwidth, $E_1 = 0.0576$. The critical value of $V$ for forming a bound state in a cubic lattice is $V_c = 3.956776$; for the trapping potential strength $V = 4.3$ used in this work the binding energy is only $E_1 = 0.06058$.

In Figs. 7.1 – 7.4, we show data for localized density profiles of multi-particle states in weak traps. The data are averaged over circular/spherical bins of unit length in the radial direction. With the Monte Carlo algorithm optimized for simulations of dilute systems, when hundreds of kinks are changed in a single elementary update, we were able to address ground state properties of very large systems (in all fixed-$N$ simulations the inverse temperature $\beta = 1/T$ was large enough to guarantee that contributions from excited states were negligible).

As the localization length rapidly increases with the number of particles, we ultimately hit the computational complexity threshold at some finite $N$. In 2D, for inter-particle repulsion strength $U = 4$, we were able to quantify properties of localized states of up to five bosons,
see Fig. 7.1. Clearly, having the inter-particle repulsion a factor of two stronger than the trap potential does not stop the system from forming a localized many-body ground state.

By fitting profile tails to the asymptotic decay of the $K_0^2(r/l_N)$ function, we deduce the ionization potential of the $N$-particle state from $I_N = 1/2ml_N^2$. It is evident that $I_N$ quickly diminishes with $N$ (this is the prime reason for why we need large systems and extremely low temperatures to reveal localized states). For $N \geq 2$ the ionization potentials can be fitted well by an exponential function $I_N \propto e^{-cN}$ with constant $c$ close to unity. This result is consistent with the mean-field picture described by the GP equation. For $U = 4$, the bare
coupling parameter $g = 1/\pi$ is smaller than unity, and the GP solution at relevant scales decays as a power law $\psi(r) = 1/4\pi gr$. This leads to an approximate relation between the particle number and localization length, $N \sim (1/2g) \ln(l_N)$, that can be used to estimate the ionization potential $\ln(I_N) = -\ln(2ml_N^2) \propto -N/4g$.

![Hard-core bosons in 2D: $L = 128, 256$](image)

**Figure 7.2.** (color online). Radial density profiles for hard-core bosons in 2D for $V = -2$ at $\beta = 16000$ (see Fig. 7.1 caption for additional details that are identical for both figures).

Trapping collapse phenomenon persists even when the on-site repulsion is taken to the ultimate hard-core (HC) limit, see Fig. 7.2. In this case, we are certainly not in the GP regime for $N = 2, 3$ since the density profile undergoes radical changes by adding one particle. Rather, we are dealing with a strongly correlated state such that when one particle is within the localization length $l$ from the trap center, the other particles are most likely to be found at a much larger distance, leading to a bi-modal structure of $n(r)$. For $N = 3$ the effects
of strong correlations are pronounced, but are less dramatic quantitatively than for \( N = 2 \). The divergence of the localization length with \( N \) in this case is much faster than for \( U = 4 \), and for \( N = 3 \) the ionization potential drops down to 0.00015, limiting our ability to monitor the crossover to the GP picture. However, given precise understanding of what happens in dilute 2D systems at large scales, there is little doubt that at zero chemical potential the ground state involves infinitely many HC particles.

![Figure 7.3](color online). Radial density profiles for two soft- and hard-core bosons in 3D for \( V = -4.3 \) at \( \beta = 10000 \). The \( L^{-3} \) level characteristic of the delocalized single-particle state is shown by bold bars. Large scale decays are fitted to the \( e^{-2r/l_2}/r^2 \) law.

We find similar results for 3D systems, see Fig. 7.3. For \( U = 1 \) (relatively weak coupling) the two-particle bound state resembles that of two bosons being placed on the same orbital, but even then the ionization potential is about a factor of six smaller than \( E_1 \). For \( U = 3 \)
we are already dealing with the ground state where positions of two particles are strongly correlated. For hard-core bosons, we certainly violate the condition (7.2), and the two-body state develops a signature bi-model shape when at short distance the two-body density profile is closely following a single particle one, see Fig. 7.3. This appears to be the generic mechanism for particles to minimize effects of strong repulsive interactions while gaining enough potential energy from the trap to remain in the localized state. The energy balance, however is extremely delicate: the ionization potential $I_2(\text{HC})$ is nearly two hundred times smaller than $E_1$!

![Figure 7.4](color online). Radial density profiles for three bosons in 2D for $U = 10$ in traps with $V = 2$ and $V = 4$ at $\beta = 4000$, showing that the state is more localized in a weaker trap.
The most intriguing question that remains unanswered by the data, is the transition between the ground state with infinitely many localized particles and a state with a few, or just one, localized particles as the range and strength of the repulsive interaction is increased, or, counter-intuitively, when the trap potential is increased. Indeed, according to expression (7.4), effects of repulsive interactions are more pronounced for smaller localization length $l$, or deeper traps. Strong-correlation effects then result in a state where one particle stays close to the trap center and effectively “screens” it out. This effect is verified and quantified in Figs. 7.4 and 7.5 using two different setups. In Fig. 7.4, we directly observe that the state of three bosons with strong on-site repulsion $U = 10$ is more delocalized in a deeper trap with $V = 4$ than in a trap with the shallow single-particle state at $V = 2$.

Higher energies for multi-particle states in a deeper trap imply that the average particle number at a given temperature and zero chemical potential must have a minimum at some value of $V$ (when $V$ is larger than $U$, one tightly localized particle can no longer fully screen the trap). Minima on the $\langle N \rangle$ curves as a function of $V$ for 2D soft-core boson with $U = 10$ are clearly seen in Fig. 7.5. As far as evidence goes, increasing trap potential for strongly repulsive bosons with $U = 10$ does not lead to the trapping collapse transition: we do not observe saturation of the $\langle N \rangle$ curves to some finite thermodynamic limit answer when the system size is increased (temperature is decreased accordingly to keep the product $TL^2 = 8$ fixed), see Fig. 7.5.

### 7.4 Conclusions

In conclusion, we have found that two- and three-dimensional finite-range potential wells, including those featuring only one weakly bound single-particle state, will localize infinitely many bosons even when repulsive inter-particle interactions are much stronger than the trapping potential. We termed this effect the trapping collapse, tracing its origin in the mean-field regime captured by the Gross-Pitaevskii equation. Evidence for trapping collapse
Figure 7.5. (color online). Average number of soft-core bosons with $U = 10$ at zero chemical potential as a function of trap strength for different system sizes and temperatures in 2D.

in the case of strong repulsive interactions was provided by path-integral Monte Carlo simulations. Future work should clarify under what conditions the trapping collapse phenomenon is replaced with localization of a finite (one?) number of particles and what are properties of systems at the transition point.
CONCLUSIONS

In the first part of this thesis, we have addressed two fundamental dynamic properties of the (2 + 1)-dimensional $O(2)$ quantum critical system.

We obtained the universal spectral densities $\Phi$ for the kinetic energy correlation function for superfluid, Mott insulator and quantum critical liquid phases in the vicinity of the QCP. Although the nature of collective modes in these phases is fundamentally different at low temperature, their $\Phi$-functions all have a resonance peak at low energy and evolve into a quasi-plateau at higher energy, in agreement with scaling predictions. In the superfluid phase, the peak is interpreted as a universal massive Goldstone resonance coming from a damped massive Goldstone mode. In the Mott insulator and quantum critical liquid phase, the existence of a pronounced peak is unexpected and we interpreted it as a massive Goldstone resonance originating from amplitude oscillations at mesoscopic length scales. The origin of this resonance requires further careful theoretical investigation.

We have also studied the universal conductivity in the low-temperature regime of the (2 + 1)-dimensional $O(2)$ quantum critical point. We have calculated the conductivity in Matsubara representation by carefully extrapolating finite system size data to the thermodynamic limit $L \to \infty$ and then taking the $T \to 0$ limit. Our result $\sigma(\infty) = 0.359(4)\sigma_Q$ is the most accurate estimate of this quantity to date. The shape of the universal conductivity function in Matsubara representation has been measured with reliable error bars and used to test the holographic theory\[11\]. The result of this comparison suggests that the theory is not compatible to our data unless the black hole temperature $T_B$ is renormlaized relative to the thermodynamic temperature. The recently proposed holographic theory, which takes ac-
count of a new relevant term in the quantum gravity theory, is consistent with our data [12]. An unambiguous proof of this new theory’s validity requires more accurate data.

In the second part of this thesis, we systematically investigated the impurity problems in quantum critical systems. We have identified two exotic impurity states.

We have established the physics of the halon, which is a special critical state of an impurity in a quantum-critical environment. The hallmark of the halon physics is that a well-defined integer charge gets fractionalized into two parts: a microscopic core with half-integer charge and a critically large halo carrying a complementary charge of $\pm 1/2$. The halon phenomenon emerges when the impurity–environment interaction is fine-tuned to the vicinity of a boundary quantum critical point (BQCP), at which the energies of two quasiparticle states with adjacent integer charges approach each other. The universality class of such BQCP is captured by a model of pseudo-spin-1/2 impurity coupled to the quantum-critical environment, in such a way that the rotational symmetry in the pseudo-spin $xy$-plane is respected, with a small local “magnetic” field along the pseudo-spin $z$-axis playing the role of control parameter driving the system away from the BQCP. On the approach to BQCP, the half-integer projection of the pseudo-spin on its $z$-axis gets delocalized into a halo of critically divergent radius, capturing the essence of the phenomenon of charge fractionalization. With large-scale Monte Carlo simulations, we confirm the existence of halons—and quantify their universal features—in O(2) and O(3) quantum critical systems.

We have found in the two- and three-dimensional vacuum-superfluid quantum critical environment, a static and attractive impurity (modeled a trapping potential) can carry divergent charge—an effect we have termed the “trapping collapse”. This physics is revealed by addressing a simple fundamental question of how many repulsively interacting bosons can be localized by trapping potentials. We find that under rather generic conditions, for both weakly and strongly repulsive particles, in two and three dimensions—but not in one-dimension!—the potential well can trap infinitely many bosons. For example, even hard-
core repulsive interactions do not prevent this “trapping collapse” phenomenon from taking place. For the weakly interacting/dilute regime, the effect can be revealed by the mean-field argument, while in the case of strong correlations the evidence comes from path-integral simulations. We also discuss the possibility of having a transition between the infinite and finite number of trapped particles when strong repulsive inter-particle correlations are increased.
BIBLIOGRAPHY


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