

Competing Orders and non-Landau-Ginzburg-Wilson Criticality in (Bose) Mott transitions

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This paper reviews a recent non-Landau-Ginzburg-Wilson (LGW) approach to superfluid to Mott insulator transitions in two dimensional bosonic lattice systems, using a dual vortex field theory.^{1),2)} The physical interpretation of conventional LGW theory of quantum criticality is re-examined and similarities and differences with the vortex picture are discussed. The “unification” of various competing (insulating) orders, and the coincidence of these orders with the Mott transition are readily understood in this formulation. Some aspects of the recent theory of “deconfined” quantum criticality, which are to an extent subsumed in this approach, are discussed. A pedagogical presentation of the “nuts and bolts” of boson-vortex duality at the hamiltonian level is included, tailored to a condensed matter audience.

§1. Introduction

Condensed matter theory continues to be challenged by the remarkable behavior of strongly correlated materials. The archetype of strong correlation physics is the Mott insulator, in which insulating behavior arises not due to the presence of filled bands (ultimately the Pauli exclusion principle), but to charge localization by strong local Coulomb interactions. Locally this physics is extremely simple, but extending it away from the atomic context, to the many-body problem is not so straightforward. The theoretical treatment of Mott insulators – and systems proximate to a Mott state – is complicated by the fact that such Mott localization reflects neither a feature of some electron-like quasiparticle spectrum, nor any kind of symmetry breaking. Thus the two workhorses of solid state physics, Landau’s Fermi liquid theory and the symmetry/order parameter description of phases of matter, are not helpful in describing the basic Mott physics.

In practice, most Mott insulators order at low temperatures, either magnetically, or by charge-order (charge density wave, stripe, etc.). These various orderings can be viewed as “competing” with one another, and with electronically-extended phases in which the Mott localization physics is not operative. Such competing orders are increasingly observable at the microscale through improvements in STM microscopy,^{3)–7)} and in crystal and surface quality. A complication for theoretical treatments of competing orders is that there are too many different charge and/or spin ordering patterns, often of considerable complexity, consistent with the sim-

ple local Mott physics requiring only single occupancy of some orbitals. Therefore we view these orders as derivative phenomena, occurring as a consequence of Mott localization, not vice-versa.

Nevertheless, competing orders seem to be an essential accompaniment to Mott localization. Indeed, there have been a number of “proofs” of late (some of which may even be rigorous!) that seem to require order of some sort in a Mott state which does not have an average electron occupation which is even per unit cell.^{8),9)} More specifically, these proofs require ground state degeneracies in large systems, which may be associated physically either to broken symmetry (presumably the usual case) or to more exotic “topological order”. Thus a minimal requirement of any reasonable theory of the Mott transition is that it should lead automatically to conventional or at least topological order.

In this paper, we discuss the SuperFluid (SF) to Mott transition in two-dimensional lattice *boson* systems.¹⁰⁾ This problem has recently become a very active experimental area with the advent of cold trapped atoms in an optical lattice.¹¹⁾ To connect it theoretically to the electronic Mott physics discussed above, one can view the bosons as tightly-bound “Cooper pairs”; the above arguments for the necessity of competing order in the insulator thus apply when the boson filling non-integral. We give a somewhat pedagogical review of recent work^{1),2)} which satisfies the above requirement of naturally describing the emergence of competing orders in the insulator, while not putting this in “by hand”. We focus on rational fillings $f = p/q$, with p, q relatively prime, and $q > 1$. This is accomplished by the use of *duality*,¹²⁾⁻¹⁴⁾ a technical transformation of the hamiltonian which has the utility of allowing one to approach the SF-Mott (putative) quantum critical point from the *superfluid* side, the opposite of the Landau-Ginzburg-Wilson (LGW) approach to superfluidity,¹⁰⁾ which expands about the normal phase in terms of the superfluid order parameter. We argue that, because of the order in the insulator, such an LGW approach is unnatural.

Thinking of the Mott transition as a Quantum Critical Point (QCP), understanding it is just the search for an appropriate continuum quantum field theory. Quantum field theories are “second quantized” descriptions of particles: point-like excitations created and annihilated by the quantum fields. LGW theory takes, loosely speaking, these particles to be the original lattice bosons. The dual approach described in this paper uses instead the *vortices* of the superfluid as these “particles”. Because it is formulated in terms of vortex excitations, this approach takes advantage of the fact that the nature of the superfluid ground state (in particular its symmetries) is *independent* of the boson filling.

What begins as a worry – the non-local nature of the phase gradient/superflow surrounding a vortex – ends up as an advantage in the approach. In the vortex formulation, this non-locality is completely accounted for by a dual gauge field A_μ , which couples minimally to the vortices. The gauge field accounts for the phase winding of the boson wavefunction upon encircling a vortex. Turned around, the vortex wavefunction must wind when encircling a boson. The phase winding due to the average boson number encircled by a minimal motion of a vortex on the lattice, is captured in the dual theory by an Aharonov-Bohm “flux” of $2\pi f$ in A_μ

through a dual plaquette.^{*)} When the bosons are at non-integer filling, this modifies the low-energy vortex dynamics in an essential way. In particular, it forces the vortices to appear in *multiplets* of q flavors, described by a vector of vortex fields, φ_ℓ , $\ell = 0 \dots q - 1$. These multiplets transform under a *projective representation* of the physical lattice symmetry group, a generalization of the ordinary notion of a representation, in which the group multiplication table is obeyed only up to phase factors, i.e. if a phase is “projected out”. An important example is the x and y lattice translations on the square lattice, which obey

$$T_x T_y = \omega T_y T_x, \quad (1.1)$$

with $\omega = e^{2\pi i f}$. This mathematically captures the Aharonov-Bohm phase described above. The modified group is dubbed a Projective Symmetry Group, or PSG.¹⁸⁾ A PSG is possible only because of the gauge nature of the vortex theory, “projection” being allowed by the lack of independent physical meaning of the local phase of the vortex field.

The PSG dictates the form of the dual effective action, similarly to how the ordinary symmetry group dictates the free energy in LGW theory. One finds (see Sec. 5)

$$\mathcal{S} = \int d^2 r d\tau \left\{ \frac{1}{2e^2} (\epsilon_{\mu\nu\lambda} \partial_\nu A_\lambda)^2 + \sum_\ell [|(\partial_\mu - iA_\mu)\varphi_\ell|^2 + \tilde{r}|\varphi_\ell|^2] + \mathcal{L}_{\text{int}} \right\}, \quad (1.2)$$

where \mathcal{L}_{int} represents quartic and higher order terms in the $\{\varphi_\ell\}$, which are strongly constrained by the PSG. The form of \mathcal{L}_{int} is, however, specific to each value of q (see Ref. 1) for a general discussion, and Sec. 6 for examples).

Eq. (1.2) describes the superfluid/Mott physics through the gauge field A_μ . For instance, the phason mode of the superfluid is described in Eq. (1.2) as the gapless transverse “photon” mode on the gauge field. The condensation of any of the φ_ℓ fields leads to a “Higgs” mass for the gauge field, corresponding to the loss of the photon and the gap in the Mott phase. Competing “charge” orders are less apparent in Eq. (1.2), but they are in fact encoded in the structure of the PSG.

In particular, the order parameters for the different charge ordering patterns occurring in Mott states can be written in terms of “density wave” amplitudes, $\rho_{\mathbf{Q}}$, describing the (complex) amplitude of a plane-wave oscillation in the charge density at wavevector \mathbf{Q} . The non-trivial vortex PSG provides a link between the vortex multiplet and spatial symmetry operations. In fact, one can explicitly construct a set of such density wave operators, with

$$\mathbf{Q}_{mn} = 2\pi f(m, n), \quad (1.3)$$

where m, n are integers. In particular, we find (see Sec. 5.3)

$$\rho_{mn} \equiv \rho_{\mathbf{Q}_{mn}} = S(|\mathbf{Q}_{mn}|) \omega^{mn/2} \sum_{\ell=0}^{q-1} \varphi_\ell^* \varphi_{\ell+n} \omega^{\ell m}. \quad (1.4)$$

^{*)} The same approach has been explored in Refs. 15)–17).

In associating the ρ_{mn} with a density, there is a general ‘form-factor’, $S(Q)$, which cannot be determined from symmetry considerations, and has a smooth Q dependence determined by microscopic details and the precise definition of the density operator.

Unlike in Landau theory, the density-wave order parameters describing the possible “competing orders” in the Mott state are quadratic rather than linear in the quantum fields of the theory. The ordering is thus “weaker” than might be expected near a LGW-type charge ordering transition, consistent with the notion that the vortex action describes the Mott transition first, and competing charge orders in the insulator only as a secondary consequence. Describing both phenomena – the loss of superfluidity and onset of charge order – simultaneously is already an achievement. It is possible because, since the φ_ℓ field carries the dual gauge charge, vortex condensation can describe both Mott physics (through the Higgs mass of A_μ when $\langle \varphi_\ell \rangle \neq 0$) and the emergent competing order arising through the ρ_{mn} . An intriguing consequence is that, even in the superfluid phase, one expects to see density wave modulations appearing in the vicinity of a localized vortex.¹⁾ Equivalent but complementary viewpoints of this non-LGW quantum criticality for the special case of half-filling have been extensively developed in recent work on “deconfined quantum criticality”¹⁹⁾ (see also Sec. 6.1.1).

This paper is written to provide a “gentler” introduction to the work of Ref. 1). To keep it pedagogical, it was not possible to go beyond this work to discuss the intended *applications* of these theoretical ideas to *electronic* systems near a *superconductor* to Mott insulator transition, with an eye to the under-doped cuprate materials. We cannot resist, however, pointing the reader toward this interesting direction. In Ref. 2), it was demonstrated that the same dual critical field theory applies to a somewhat more microscopically faithful representation of strong electronic pairing, the doped quantum dimer model.²⁰⁾ The authors believe that it indeed applies more generally to any two-dimensional *clean* singlet superconductor to Mott insulator transition, in which the gap in the superconducting state is complete. Most recently, it was proposed that the observation of “checkerboard” charge correlations near vortices in BSCCO by Hoffman *et al.*,²¹⁾ is indicative of similar physics. This suggestion was used to extract some bounds on the inertial mass of a vortex from these experiments.²²⁾ The reader should note that, because the cuprate materials are gapless, d-wave superconductors, this interpretation goes boldly beyond the existing theory. Theoretical work to directly address the additional quasiparticle physics in gapless superconductors is ongoing.

The remainder of this paper is organized as follows. In Sec. 2, we describe the general structure of simple models of lattice bosons, which contain superfluid to Mott transitions. Sec. 3 describes the conventional LGW theory of the SF-Mott QCP for *integer* boson filling, emphasizing that it should be understood as based upon elementary particle/hole excitations of the Mott state. Sec. 4 describes the dual vortex description of this conventional integral filling Mott transition, including a pedagogical description of hamiltonian boson-vortex duality. Sec. 5 applies the dual formulation to non-integral Mott transitions, and describes the origin of the main results summarized in this introduction. Finally, Sec. 6 details some specific

predictions of the theory for $f = 1/2$, which provides an example and view to “deconfined criticality”, and for $f = 1/3$, which does not.

§2. Bose Mott Insulators

2.1. Physics and model

The simplest systems that can exhibit a Mott transition between states with extended and localized carriers are those composed of interacting lattice bosons, the extended states being superfluids/superconductors, and the Mott states being generally charge ordered away from integer boson fillings. An exciting experimental development of late is the direct realization of such models of cold atomic bosons confined to an optical lattice. These will likely turn out to provide the cleanest experimental tests of theoretical approaches to this simplest Mott problem. Conceptually, a symmetry-equivalent problem arises if fermions (e.g. electrons) are strongly bound into bosonic Cooper pairs. This is not clearly realized in any simple electronic material. One may expect, however, that a bosonic theory of this sort will properly describe the *universal* low energy properties of an electronic system in the vicinity of a superconductor to Mott insulator transition, provided that both the superconductor and insulator are “bosonic”. More precisely, we believe it clearly applies when the superconductor should be clean (strictly speaking, *superclean*) and with a full gap (e.g. s-wave) to unpaired quasiparticle excitations, and the Mott insulator should exhibit only charge (e.g. not spin) order. Similar theories likely apply more generally to other superconductor to Mott insulator transitions, but are beyond the scope of this paper.

We concentrate now on purely bosonic Mott transitions. We use a “rotor” representation for the bosons, with phase operators $\hat{\phi}_i$ and conjugate number operators \hat{n}_i where i runs over the sites of the direct lattice. These operators obey the commutation relation

$$[\hat{\phi}_i, \hat{n}_j] = i\delta_{ij}. \quad (2.1)$$

One may consider a variety of geometries, but we will focus here upon the simple square lattice.

A simple boson hamiltonian in the class of interest has the structure

$$\mathcal{H} = -t \sum_{i\alpha} \cos(\Delta_\alpha \hat{\phi}_i) + U \sum_i (\hat{n}_i - \bar{n})^2 + \mathcal{H}', \quad (2.2)$$

where t represents a nearest-neighbor boson hopping amplitude, and U an on-site boson repulsion. We denote by Δ_α the discrete lattice gradient in the α direction. Additional more complicated off-site terms are included in the unspecified contribution to the hamiltonian, \mathcal{H}' (but see below). For now we require only that it respect the symmetries of the underlying lattice, boson conservation, and locality (e.g. the amplitude for hopping between far away sites should decay sufficiently rapidly with distance).

Eq. (2.2) may be studied in the grand canonical ensemble, i.e. at fixed chemical potential ($2U\bar{n}$). However, one may equally well consider instead the canonical

ensemble with fixed boson number (average filling f). We will typically do the latter, except in Secs. 2.2, 2.3, and the first part of Sec. 3, where we work at fixed chemical potential.

2.2. Mott states at integral filling

Neglecting terms in \mathcal{H}' , the zero temperature phase diagram of \mathcal{H} is well-known.¹⁰⁾ It takes the schematic form in Fig. 1. For $t/U \ll 1$, the system is in a Mott insulating ground state, with $\langle \hat{n}_i \rangle = N$, the integer nearest to \bar{n} , on every site. This phase persists inside the “lobes” drawn in the figure. There is a gap to the lowest-lying excited states, which may be thought of as single extra/missing bosons (which delocalize into plane-waves). For large t/U , the ground state is a superfluid (**SF** in the figure), with $\langle e^{i\hat{\phi}_i} \rangle = \Psi_{sf} \neq 0$, and the density $f = \langle \hat{n}_i \rangle$ varies smoothly with parameters in an unquantized fashion. There is no excitation gap, and the lowest-lying excitations are acoustic “phonons” or “phasons”, the Goldstone modes of the broken $U(1)$ symmetry of the superfluid.

2.3. Mott states at non-integral filling

We now return to the shaded regions of the phase diagram in Fig. 1, where states with different boson density are nearly degenerate. Indeed, in the simple model with $\mathcal{H}' = 0$, for $\bar{n} = N + 1/2$, states with any average density between N and $N + 1$ are degenerate. For $t/U = 0$, the eigenvalue of $\hat{n}_i = N$ or $\hat{n}_i = N + 1$ can be independently chosen on each site. The omitted terms in \mathcal{H}' will then clearly determine the nature of the ground states appearing in the shaded region. Generally, Mott insulating states appear at rational fractional fillings, $f = p/q$, with p, q relatively prime. For $q > 1$, these are boson “crystals” or charge density waves. Mott states with increasing q are expected to require longer-range interactions in \mathcal{H}' for their stabilization.

For example, in the vicinity of $\bar{n} = N + 1/2$, we can adopt a pseudo-spin description, with $S_i^z = \hat{n}_i - N - 1/2 = \pm 1/2$. In the limit of $U \rightarrow \infty$ (or $t/U \ll 1$), one can then replace

$$\mathcal{H} \rightarrow -t \sum_{\langle ij \rangle} \left(S_i^+ S_j^- + S_i^- S_j^+ \right), \quad (2.3)$$

with $\langle ij \rangle$ indicating the sum is taken

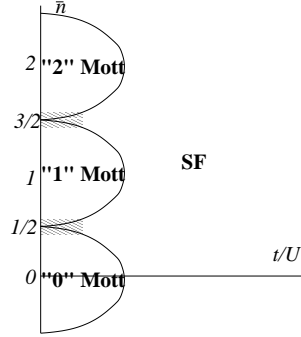


Fig. 1. Schematic phase diagram of boson rotor model, with on-site interactions only. The shaded regions indicate where there is a large near-degeneracy of states with different boson densities, and the system is highly susceptible to off-site interactions.

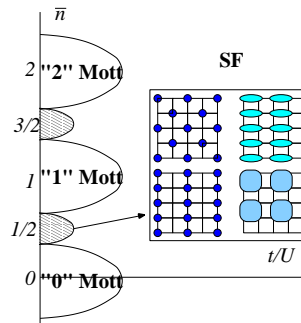


Fig. 2. Schematic phase diagram with off-site interactions. Some representative Mott insulating states with $\langle \hat{n}_i \rangle = N + 1/2$ are shown.

over nearest-neighbor sites, and the conventional definitions of spin-1/2 raising and lowering operators. This term tends to split the degeneracy of boson states in favor of a delocalized superfluid. Terms in \mathcal{H}' can compete with this term for small t , splitting the degeneracy instead in favor of a non-trivial Mott state. For instance, one may take

$$\mathcal{H}' = J_z \sum_{\langle ij \rangle} S_i^z S_j^z + J'_z \sum_{\langle\langle ij \rangle\rangle} S_i^z S_j^z - K \sum_{\square} \left(S_i^+ S_j^- S_k^+ S_l^- + \text{h.c.} \right) + \dots \quad (2.4)$$

Here $\langle\langle ij \rangle\rangle$ indicates a sum over next-nearest-neighbors, and the \square a sum over four site plaquettes (with sites i, j, k, l labelled clockwise around the plaquette). For $t \ll \min\{J_z, J'_z, K\}$, a variety of Mott states occur in such a model, including “solids” and “valence bond solids” as shown in Fig. 2. The figure also shows a schematic phase diagram in which Mott states with $q = 2$ are stable. More complex phases (with $q > 2$) have been observed in similar models in the literature.²³⁾

§3. “Integral” Mott-Superfluid transitions: LGW theory as Bose condensation

It is well-known that the quantum phase transitions across the phase boundaries in Fig. 1 are described by LGW theories.¹⁰⁾ On symmetry grounds, this is understandable, since the assumptions underlying Landau’s theory are valid. In particular, the integer filling Mott states, being unique, and having the full symmetry of the underlying hamiltonian and only short-range correlations, may be regarded as truly “disordered”. The superfluid is the “ordered” phase, its symmetry group (the lattice space group) being a subgroup of the symmetry group of the Mott state (the direct product of the lattice space group and the $U(1)$ boson number conservation symmetry). A LGW-style expansion of the effective action in terms of the superfluid order parameter Ψ and its derivatives indeed seems to describe the quantum critical points.

It is instructive, however, to understand these transitions more physically. We will demonstrate that the physical content of the LGW theory is Bose-Einstein condensation of “particle” and/or “hole” excitations of the Mott state. To that end, let us think about the elementary excitations in that phase. For $U/t \gg 1$, the ground state is simply

$$|GS\rangle = \prod_i (b_i^\dagger)^N |0\rangle, \quad (3.1)$$

where $b_i = e^{-i\hat{\phi}_i}$ is the boson annihilation operator in the rotor formulation, and $|0\rangle$ is the state of “no bosons” (zero rotor angular momentum), $\hat{n}_i |0\rangle = 0$ (note that eigenstates of \hat{n}_i exist with negative as well as non-negative integer eigenvalues in the rotor formulation). In the same limit, the lowest excited states are “particles” and “holes” with one extra or missing boson,

$$|p_i\rangle = b_i^\dagger |GS\rangle, \quad (3.2)$$

$$|h_i\rangle = b_i |GS\rangle. \quad (3.3)$$

For $t/U = 0$ strictly, the particle and hole energies (relative to the ground state) are

$$E_p^{(0)} = 2U(N + \frac{1}{2} - \bar{n}), \quad E_h^{(0)} = 2U(\bar{n} + \frac{1}{2} - N). \quad (3.4)$$

For $0 < t/U \ll 1$, these states will develop dispersion. By considering the first order splitting of the degenerate manifold of particle or hole states (degeneracy associated with the site of the particle or hole), one obtains

$$E_{p/h} = E_{p/h}^{(0)} - 2t(\cos k_x + \cos k_y) \approx \Delta_{p/h} + \frac{k^2}{2m}, \quad (3.5)$$

where we have Taylor expanded around the minimum at $\mathbf{k} = \mathbf{0}$, giving $m = 1/(2t)$. The minimum energy excitation is then a particle or hole, for $\bar{n} > N$ or $\bar{n} < N$, respectively. The excitation gap, $\Delta_{p/h}$, is

$$\Delta_{p/h} = 2U(\frac{1}{2} \mp (\bar{n} - N)) - 4t, \quad (3.6)$$

to this order. A simple-minded extrapolation of this formula to larger t suggests that the excitation gap for particles or holes will vanish once $t/U \geq (\frac{1}{2} - |\bar{n} - N|)/2$. Though this $O(1)$ value is well beyond the region of validity of the expansion (except for $|\bar{n} - N| \approx \frac{1}{2}$, where it is invalid for other reasons, to be discussed below), it does suggest a simple physical picture of the transition to the superfluid, as a ‘‘condensation’’ of these particles or holes. For $\bar{n} > N$, the particles condense, while for $\bar{n} < N$ the holes do. Precisely at $\bar{n} = N$, both condense simultaneously. This latter case automatically applies in the canonical ensemble if the filling f is fixed to be integral.

We will now show that such particle/hole condensation is the physical content of the LGW theory. While it is possible to derive a field theory of this condensation from \mathcal{H} , we instead just write it down based on this simple physical picture. We model the particle and hole excitations by fields $p(\mathbf{x}, \tau), h(\mathbf{x}, \tau)$ respectively, in the imaginary time (τ) path integral. The weight in the path integral is, as usual, the Euclidean action,

$$\mathcal{S} = \int d\tau d^2x [p^\dagger(\partial_\tau + E_p - \frac{1}{2m}\nabla^2)p + h^\dagger(\partial_\tau + E_h - \frac{1}{2m}\nabla^2)h - \lambda(p^\dagger h^\dagger + ph) + \dots]. \quad (3.7)$$

Here we have included a term λ which creates and annihilates particles and holes together in pairs, which is expected since this conserves boson number. Microscopically this term arises from the action of the hopping t on the naïve ground state, which creates particle-hole pairs on neighboring sites, so $\lambda \sim O(t)$ (the spatial dependence is unimportant for the states near $\mathbf{k} = \mathbf{0}$). We have neglected – for brevity of presentation – to write a number of higher order terms involving four or more boson fields, representing interactions between particles and/or holes, and other boson number-conserving two-body and higher-body collisional processes. Note that the dependence upon t/U in Eq. (3.7) arises primarily through implicit dependence of $E_{p/h}$.

Eq. (3.7) can be systematically analyzed by diagonalizing the quadratic form involving p, h . The qualitative features can be understood even more simply by considering simple limits. First, suppose $\bar{n} > N$, so $E_p < E_h$. Upon increasing t/U , then, at some point $E_p \rightarrow 0$ while $E_h > 0$. Then the holes are still gapped, and the h field can be integrated out order by order in λ and higher order terms, encountering no vanishing energy denominators. One has then an effective action for the remaining particle field p ,

$$\mathcal{S} = \int d\tau d^2x \left[p^\dagger (\partial_\tau + \tilde{E}_p - \frac{1}{2m} \nabla^2) p + u(p^\dagger p)^2 + \dots \right], \quad (3.8)$$

with $\tilde{E}_p \approx E_p - O(\lambda^2/E_h)$ a renormalized particle gap. This is exactly the well-known effective action for the superfluid-Mott transition, which has an LGW form with the “order parameter” being the particle field p . The single ∂_τ derivative is well-understood and present because particle annihilation becomes particle creation under time-reversal, and leads to so-called $z = 2$ behavior of the QCP.

The case of $\bar{n} < N$ can be understood similarly with the roles of particles and holes interchanged. The remaining case of $\bar{n} = N$ (the tips of the lobes in Fig. 1) is slightly different. In that case, both particles and holes become gapless together as t/U is increased. Thus we may expect a “relativistic” theory in which particles and holes appear in a sense as particles and antiparticles. This is seen by changing variables to the linear combinations

$$\Psi = \frac{1}{\sqrt{2}}(p + h^\dagger) \quad \Xi = \frac{1}{\sqrt{2}}(p - h^\dagger). \quad (3.9)$$

Writing $E_p = E_h \equiv E_0$, one finds that (taking $\lambda > 0$ without loss of generality) the quadratic form for Ψ becomes unstable before that of Ξ , and one can therefore integrate out Ξ to obtain

$$\mathcal{S} = \int d\tau d^2x \left[\Psi^\dagger \left(-\partial_\tau^2 - \frac{1}{2m} \nabla^2 + r \right) \Psi + u(\Psi^\dagger \Psi)^2 + \dots \right], \quad (3.10)$$

with $r \approx E_0 - \lambda$. Apart from a trivial space-time anisotropy, Eq. (3.10) is exactly the classical LGW free energy of a three-dimensional normal-superfluid transition. Thus the two LGW actions, Eqs. (3.8,3.10), usually denoted as particle-hole asymmetric and symmetric theories, respectively, are indeed physically equivalent to particle or particle+hole condensation.

§4. “Integral” Mott-Superfluid transitions: vortex condensation theory

As discussed in the introduction, a quantum field theory description of the QCP would appear to require only some pointlike “particles” described by the quantum fields (as creation/annihilation operators). On the Mott side of the transition, particle and/or hole excitations provide these, and their condensation precisely coincides with LGW theory. On the superfluid side, there is another quite different pointlike “particle” excitation: a vortex or anti-vortex. This is specific to two-dimensional superfluids, since a vortex becomes a line defect in three dimensions.

It is natural then to try to describe the Superfluid-Mott transition, coming from the superfluid side by a field theory for vortices. Provided time-reversal symmetry \mathcal{T} is unbroken, one should expect such a field theory to be relativistic, since vortices and anti-vortices are interchanged by \mathcal{T} (note that this is independent of the presence or absence of particle/hole symmetry in the boson system). One may worry that a vortex is a non-local object, with a power-law tail of superflow surrounding it extending to infinity. Perhaps this invalidates its use as a particle?

4.1. Duality

This worry is resolved by *duality*, which is a rigorous mathematical mapping of the original rotor boson model to one of vortices. We will see that all the non-locality of the vortex is taken into account by a *non-compact* $U(1)$ gauge field. The dual formulation is mathematically analogous to a lattice $U(1)$ Higgs theory of particle physics, or a lattice classical three-dimensional Ginzburg-Landau theory for a superconductor (charged superfluid).

Boson-vortex duality is extensively covered in the literature. It is however often a confusing topic for students and senior researchers alike. This is because certain stages of the duality mapping are usually performed in a rather non-rigorous fashion, involving so-called ‘‘Villain potentials’’, fudging with the time-continuum limit in the path integral, and other similar manipulations. In reality this sloppiness is unimportant, since the usefulness of duality does not lie in the quantitative analysis of specific microscopic models, but in its application to universal phenomena. Nevertheless, it seems anathema to those trained in the more rigorous solid state physics tradition rather than the effective field theory approach originating from statistical mechanics.

For this reason we will present here what to our mind is the simplest and most rigorous possible version of $U(1)$ duality, performed at the hamiltonian level. This proceeds in several steps. The first, completely rigorous and explicit step, contains the essence of the duality mapping. It is simply a change of variables from boson number and phase $\hat{n}_i, \hat{\phi}_i$ living on the direct lattice sites, to new ‘‘electric field’’ and ‘‘vector potential’’ variables, $E_{a\alpha}, A_{a\alpha}$, living on the links of the dual lattice (We use a, b, c to label sites of the dual lattice, and $\alpha, \beta = 1, 2$ to label links of the dual square lattice in the x, y directions, respectively):

$$E_{a\alpha} = \frac{(\epsilon_{\alpha\beta} \Delta_\beta \hat{\phi})_a}{2\pi}, \quad (4.1)$$

$$\hat{n}_i = \frac{(\epsilon_{\alpha\beta} \Delta_\alpha A_\beta)_i}{2\pi}. \quad (4.2)$$

Geometrically, the oriented electric field on a link of the dual lattice is taken to equal $1/(2\pi)$ times the phase difference between the phase $\hat{\phi}_i$ to immediately to the right (using the orientation of the field) of the dual link and the phase $\hat{\phi}_j$ immediately to the left of this dual link. The electric field $E_{a\alpha}$ is thus a periodic variable, with $E_{a\alpha} \leftrightarrow E_{a\alpha} + 1$. The dual vector potential $A_{a\alpha}$ is a discrete field, i.e. has eigenvalues of 2π times integers. It is implicitly defined by Eq. (4.2) so that its lattice curl – the counter-clockwise circulation around a dual plaquette – is 2π times the boson

number inside this dual plaquette. The $A_{a\alpha}$ variables have a “gauge” redundancy: the vector potential can be shifted by any $2\pi \times$ integer gradient, $A_{a\alpha} \rightarrow A_{a\alpha} + \Delta_\alpha \chi_a$ (with $\chi_a \in 2\pi\mathcal{Z}$) without changing \hat{n}_i . To achieve a one-to-one mapping of $A_{a\alpha}$ to \hat{n}_i , one can “fix a gauge” in numerous ways, e.g. for Coulomb gauge, $\Delta_\alpha A_{a\alpha} = 0$.

It is straightforward to check (by comparing the commutator of the left-hand side of Eq. (4.1) and the right-hand side of Eq. (4.2) with the commutator of the right-hand side of Eq. (4.1) and the left-hand side of Eq. (4.2)), that the dual electric and vector potential variables are canonically-conjugate:

$$[A_{a\alpha}, E_{b\beta}] = i\delta_{ab}\delta_{\alpha\beta}. \quad (4.3)$$

Furthermore, the expression in Eq. (4.1) implies a constraint:

$$\Delta_\alpha E_{a\alpha} \in \mathcal{Z}, \quad (4.4)$$

i.e. the lattice divergence of the dual electric field is an integer (a non-zero value being “allowed” due to the periodicity of the $\hat{\phi}_i$ and $E_{a\alpha}$ variables). Physically, this integer can be identified with the vorticity. This can be seen by considering the line sum of $\Delta_\alpha \hat{\phi}_i$ around some area. In an abuse of the continuum notation,

$$\oint \nabla \hat{\phi} \cdot d\mathbf{l} = 2\pi \oint \mathbf{E} \cdot d\hat{\mathbf{n}} = 2\pi \int d^2x \Delta_\alpha E_{a\alpha}, \quad (4.5)$$

so that the phase winding around some area, in units of 2π , just counts the total divergence of $E_{a\alpha}$ inside this area, i.e. the net dual “charge” inside this area.

With full rigor,^{*)} the hamiltonian can be rewritten as

$$\mathcal{H} = -t \sum_{a\alpha} \cos 2\pi E_{a\alpha} + \frac{U}{(2\pi)^2} \sum_i ((\epsilon_{\alpha\beta} \Delta_\alpha A_\beta)_i - 2\pi\bar{n})^2. \quad (4.6)$$

Already without further manipulation, Eq. (4.6) appears very similar to an electromagnetic hamiltonian ($\propto E^2 + B^2$). It is, however, inconvenient to work with since $A_{a\alpha}$ is a discrete, $2\pi \times$ integer-valued field. To understand how to remedy this deficiency, it is instructive to express the first term in Eq. (4.6) in the $A_{a\alpha}$ basis. Since the electric field is conjugate to the vector potential, this cosine is just a “shift” operator for the $A_{a\alpha}$ field. Hence we can write

$$-t \cos 2\pi E_{a\alpha} = -t \sum_{A_{a\alpha}} (|A_{a\alpha} + 2\pi\rangle \langle A_{a\alpha}| + |A_{a\alpha}\rangle \langle A_{a\alpha} + 2\pi|). \quad (4.7)$$

One can think of the basis for the Hilbert space of a single link of the dual lattice as consisting of $2\pi \times$ integer-spaced “sites” along a “line” $A_{a\alpha}$ -space. The original boson-hopping term on a link of the direct lattice is just a tight-binding hopping hamiltonian for the “line” associated to the dual link crossing this direct link.

The analogy to a tight-binding model thereby suggests a means of removing the discrete constraint on $A_{a\alpha}$. We can do this by simply replacing the tight-binding

^{*)} Some small additional care needs to be taken for finite systems with periodic boundary conditions, in which case additional c-number terms should be added to the left-hand side of Eq. (4.2).

model by a continuum one of a particle in a periodic potential, strategically chosen so that the lowest band is (arbitrarily) well-approximated by a tight-binding band, well-separated from higher energy states. This amounts to replacing

$$-t \cos 2\pi E_{a\alpha} \rightarrow \frac{1}{2\kappa} E_{a\alpha}^2 - \tilde{t} \cos A_{a\alpha}, \quad (4.8)$$

and allowing $A_{a\alpha}$ to take arbitrary continuous real values. The tight-binding limit is recovered for $\tilde{t}\kappa \gg 1$. One can then adjust \tilde{t}, κ to achieve the desired tight-binding matrix element t between nearly-localized levels in neighboring wells of the \tilde{t} potential. We do not do this explicitly here, since we will not use it in the following. It can, however, be achieved, by taking $\tilde{t}, \kappa^{-1} \gg U$, to arbitrary desired accuracy.

We are left with the hamiltonian

$$\mathcal{H} = \sum_{a\alpha} \left[\frac{1}{2\kappa} E_{a\alpha}^2 - \tilde{t} \cos A_{a\alpha} \right] + \tilde{U} \sum_i ((\epsilon_{\alpha\beta} \Delta_\alpha A_\beta)_i - 2\pi\bar{n})^2, \quad (4.9)$$

with $\tilde{U} = \frac{U}{(2\pi)^2}$. This must be supplemented by the commutation relations, Eq. (4.3), and the constraint, Eq. (4.4).

Eq. (4.9) is clearly a $U(1)$ gauge theory, but the presence of ‘‘vortex’’ variables is not immediately apparent. In fact, they are implicit in the constraint, Eq. (4.4), which can be regarded as Gauss’ law (in the dual electromagnetic analogy). Sites with non-zero $\Delta_\alpha E_{a\alpha}$ thus correspond to dual charges – physical vorticities. Though no explicit vortex variables appear, they are un-necessary: the locations of all (dual) charges can be determined from the electric field lines.

It is nevertheless useful (and conventional) to introduce redundant vortex variables. In particular, we introduce an auxiliary Hilbert space of integer rotor states, eigenvectors of $N_a \in \mathcal{Z}$, and conjugate variables θ_a , with $[N_a, \theta_b] = i\delta_{ab}$ as usual. These states are introduced only to redundantly label the vortex positions. So we require

$$\Delta_\alpha E_{a\alpha} = N_a. \quad (4.10)$$

For this to be consistent with the hamiltonian action in the expanded Hilbert space, we must ensure that the $-\tilde{t} \cos A_{a\mu}$ term, which changes the electric divergence on neighboring sites, also increment the new rotor variables. This is accomplished by modifying $A_{a\alpha} \rightarrow A_{a\alpha} - \Delta_\alpha \theta_a$. Making this shift, one sees that the hamiltonian in Eq. (4.9) is completely equivalent to the more conventional form

$$\mathcal{H} = \sum_{a\mu} \left[\frac{1}{2\kappa} E_{a\mu}^2 - \tilde{t} \cos(\Delta_\alpha \theta_a - A_{a\mu}) \right] + \tilde{U} \sum_i ((\epsilon_{\mu\nu} \Delta_\mu A_\nu)_i - 2\pi\bar{n})^2, \quad (4.11)$$

combined with the constraint in Eq. (4.10).

4.2. Phases in the dual formulation, for integer f

For integer \bar{n} , we may remove the dual ‘‘background flux’’ $2\pi\bar{n}$ in the last term in Eq. (4.11) by the shift $A_{a2} \rightarrow A_{a2} + 2\pi f a_x$ (with (a_x, a_y) the coordinate of site a). Here we are guaranteed $f = \bar{n}$ by particle-hole symmetry of the on-site rotor

model. More generally, working in the canonical ensemble with fixed filling f , this shift by construction takes account exactly of the average dual flux in $A_{a\alpha}$ – the fluctuations around this shifted around are zero by this choice. One thus has just a theory of lattice electromagnetism coupled to a “charged scalar” field $\psi_a = e^{-i\theta_a}$. It may equally well be thought of as a Ginzburg-Landau-like theory of a dual lattice “superconductor” with “pair field” ψ_a .

From these analogies, one expects two phases. In the gauge theory language, there is a “Coulomb phase” or “dielectric”, in which the charged particle is gapped and can be integrated out. A simple limit of this phase is obtained by taking $\tilde{t} = 0$. In this limit, N_a is a constant of motion on each dual lattice site. Because of the Gauss’ law constraint, Eq. (4.10), the ground state is clearly obtained for $N_a = 0$, i.e. no vortices present. Individual vortices can be introduced anywhere in the system and in this limit have no dynamics, but due to the constraint, an energy cost which is logarithmic in system size (due to the dual electric field lines decaying as $1/r$ far from the vortex). Clearly this is the physical superfluid phase in the direct language. As in any superfluid, we expect a phason or Goldstone mode. This corresponds to the gapless linearly dispersing transverse photon of the dual electromagnetism (there is only a single polarization in two spatial dimensions). Going back to the duality mapping, it is straightforward to see that small \tilde{t} corresponds to a large “tight-binding bandwidth” for $A_{a\alpha}$, i.e. a large direct boson hopping amplitude, where we indeed expect a superfluid state.

The other phase is a “Higgs phase” or dual “superconductor”, in which the ψ_a particle is condensed. In this “Higgs” phase the photon is gapped, and indeed there is an energy gap to all excitations. Moreover, there is no broken symmetry: the condensate amplitude $\langle \psi_a \rangle$ is not gauge invariant and the vortex condensation does not itself represent an order parameter for any broken symmetry. This then corresponds to the featureless Mott insulating state in the direct picture.

4.3. Continuum field theory (for integer f)

For integer f , a rather naïve continuum limit is possible, due to the ability to transform away the background “flux” in Eq. (4.11). It is instructive, paralleling the logic used above to derive the LGW theory coming from the Mott state, however, to think more physically in terms of the vortex excitations. We imagine coming from the superfluid state, by increasing \tilde{t} starting from a small value. At first pass, we will neglect the fluctuations of $A_{a\alpha}, E_{a\alpha}$.

For $\tilde{t} = 0$, the ground state $|0\rangle$ clearly has $N_a = 0$, and corresponds to the vortex “vacuum”. The lowest excited single vortex states correspond to $N_a = \pm 1$ on an (arbitrary) single site a , which we denote

$$|a+\rangle = \psi_a^\dagger |0\rangle = e^{i\theta_a} |0\rangle, \quad (4.12)$$

$$|a-\rangle = \psi_a |0\rangle = e^{-i\theta_a} |0\rangle. \quad (4.13)$$

These states are elementary in that any vortex number configuration can be built from them by superposition. Each such state has a logarithmically-divergent energy, since the Gauss’ law constraint, Eq. (4.10), requires $E_{a\alpha} \sim 1/r$ far from the vortex: this is just the usual logarithmic vortex energy coming from the long-range superflow.

We will return to this point below.

First order degenerate perturbation theory in \tilde{t} gives an effective single-particle tight-binding model amongst the $|a_{\pm}\rangle$ states, and hence some plane-wave eigenstates with energy dispersion. One may now follow the same logic as in Sec. 3, with the vortex/anti-vortex states playing the analogous roles to the particle/hole excitations in the Mott phase. Time-reversal symmetry guarantees that these have the same excitation gap. Recognizing that these states carry the dual gauge charge, and allowing for fluctuations in the $A_{a\alpha}, E_{a\alpha}$ fields, one thereby arrives (following the same methodology as in Sec. 3, using the coherent state path integral, and the standard path integral Trotterization of electromagnetism) at the continuum action

$$\mathcal{S}_{dual} = \int d\tau d^2x \left[\frac{1}{2e^2} (\epsilon_{\mu\nu\lambda} \partial_\nu A_\lambda)^2 + |(\partial_\mu - iA_\mu)\varphi|^2 + \tilde{r}|\varphi|^2 + \tilde{u}|\varphi|^4 + \dots \right]. \quad (4.14)$$

Here for compactness, we have neglected to write unimportant space-time anisotropies (constant scale factors) that appear between space and time derivatives, and spatial (electric) and temporal (magnetic) fluxes, writing simply three-dimensional coordinates (τ, x, y) and indices $\mu, \nu, \lambda = 0, 1, 2$. The anisotropies do not lead to any additional physics, and are expected to be irrelevant or redundant at the QCP. New coupling constants $\tilde{r}, \tilde{u}, e^2$ have been defined in the continuum action.

Eq. (4.14) is identical to the classical free energy of a three-dimensional Ginzburg-Landau theory for a superconductor. The duality between this form and Eq. (3.10), the classical three-dimensional XY free energy, was established in Ref. 12). Because the LGW form, Eq. (3.10), does not involve any gauge field, it is of more practical (analytical and numerical) use in this case. Nevertheless, we emphasize that both the LGW and dual actions are descriptions of the *same* critical point. Qualitatively the same physics can be extracted from either form, though they will yield different quantitative results from approximate treatments.

It is instructive to review how the measures of charge localization are encoded in Eq. (4.14). The boson creation operator, b_i^\dagger , is a 2π flux insertion operator in the dual formulation, i.e. it creates a *space-time monopole* with $\partial_\mu B_\mu = 2\pi\delta^{(3)}(x, \tau)$, where the dual space-time magnetic flux $B_\mu = \epsilon_{\mu\nu\lambda}\partial_\nu A_\lambda$ is physically the boson 3-current. By looking at monopole correlators, therefore, one can discern the presence or absence off-diagonal long-range order, or the presence or absence of a gap. The superfluid density ρ_s and compressibility κ measure the response to external physical vector and scalar potentials, respectively. These physical potentials couple to the boson 3-current, and hence ρ_s and κ are obtained from correlation functions of the A_μ gauge field. The lesson to be learned here is that *all* Mott/Superfluid properties are encoded in the properties of the gauge field A_μ , not directly in the dual “order parameter” φ (which anyway is not gauge-invariant – See Sec. 4.3.1 for further related discussion).

A studious reader may wish to try the following illustrative exercise: calculate the critical behavior of the superfluid density using the dual form in the “random phase approximation”. This can be done by introducing an external gauge field,

A_μ^{ext} , which couples to the physical electromagnetic current,

$$\mathcal{S} \rightarrow \mathcal{S} - i \int d\tau d^2x A_\mu^{\text{ext}} \epsilon_{\mu\nu\lambda} \partial_\nu A_\lambda. \quad (4.15)$$

Neglecting the $|\varphi|^4$ term, integrate out φ at quadratic level in A_μ , then integrate out A_μ itself, to obtain the coefficient of $(P_T A_\mu^{\text{ext}})^2$ (P_T is a transverse projection operator), which is proportional to ρ_s . One may compare the manner in which this vanishes with \tilde{r} with the mean-field LGW prediction for how ρ_s vanishes with r in Eq. (3.10).

4.3.1. Logarithmic vortex potential and bound states

A careful reader may be troubled by the notion of using a vortex as an elementary excitation, since, in the superfluid state, it has a logarithmically divergent energy (in the system size). A partial answer to this question is that any neutral collection of equal numbers of vortices and antivortices has finite energy. However, it is clear that a vortex and anti-vortex attract each other, and will form a bound state, with infinite (logarithmically) binding energy. On increasing \tilde{t} within the superfluid state, one may suspect that such a vortex/anti-vortex pair excitation will condense before individual vortices do.

In fact, more careful thought is needed. In the “relativistic” theory of Eq. (4.14) (or the lattice hamiltonian, Eq. (4.11)) vortices and anti-vortices are not separately conserved. Indeed, the action of \tilde{t} on the ground state creates them in pairs on nearest-neighbor links (compare to the λ term in Eq. (3.7)). Thus the number of such “bound states” is not a conserved quantity, and consequently there is no sharp phase transition associated to their “condensation” – any “creation operator” for these bound states has a non-vanishing expectation value for all $\tilde{t} > 0$, unless it is finely tuned. Thinking spectrally, were such a single neutral bound state to approach zero energy upon increasing \tilde{t} , it would be expected to have an *avoided crossing* with the ground state, because of the non-zero matrix element between the naïve ground state and the state with one excited bound pair.

More generally, Eqs. (4.14,4.11) have *no internal symmetries*, only space-time symmetries and “gauge invariance” which is not a symmetry at all but embodies a dynamical constraint. Phase transitions in these models are then expected to be either associated with the development of a Higgs mass for the gauge field, or by breaking of spatial lattice symmetries (the latter not being expected to occur for $f \in \mathcal{Z}$).

Nevertheless, it is a reasonable physical question to ask why it is that a description in terms of elementary individual vortex excitations is appropriate when these objects are always infinitely strongly bound on the superfluid side of the transition. The answer is that, as the Superfluid-Mott QCP is approached, the interaction between vortices is becoming progressively more and more “screened” by virtual fluctuations of vortex/anti-vortex pairs. This can be seen, for instance, from the fact that the superfluid density vanishes at the QCP. Alternatively, just from scaling, at the critical point, the interaction between two static external dual “test charges” separated a distance r behaves like $1/r$, not logarithmically. A screened interaction

prevails on scales smaller than the correlation length, which diverges as the QCP is approached.

§5. Non-integral Mott-Superfluid transitions: vortex theory

Having understood the direct and dual formulations of the integral Superfluid-Mott transition, we turn to the non-integral case. We will concentrate on rational mean fillings, $f = p/q$, with p, q relatively prime, and $q > 1$ but not too large. We assume that sufficient interactions are present to stabilize a “crystalline” Mott insulating state at such a density. We must then analyze Eq. (4.11), with $\bar{n} \approx p/q$.

If we attempt to approach the problem from an LGW perspective, there is a fundamental difficulty: neither the Mott insulator or Superfluid are “disordered” phases, the former breaking space-group symmetries of the lattice, and the latter breaking the $U(1)$ boson conservation symmetry. Landau theory can only describe the transition from one of these states to an even more symmetry-broken phase, which then seems to require an intermediate phase between the two.

Taking a more physical point of view, we can search for pointlike excitations in either phase that could provide the degrees of freedom for a critical quantum field theory. Unfortunately, on the Mott side, the nature of the elementary excitations would seem to be very specific to the particular Mott state under consideration. All the Mott phases presumably include extra/missing boson “particles”, as well as domain wall and other discrete topological excitations particular to the precise type of boson density order in the ground state. The extra/missing boson “particles” could provide the variables for some QCP, but one expects condensation of such particles not to disrupt the density-wave order of the Mott state, leading to a “supersolid” rather than a true superfluid. As such states appear to be even more exotic than superfluids and Mott insulators, we will not explore that possibility further. A theory based on topological excitations of particular Mott states is possible, but much more limited in scope (see Ref. 1), Sec. ?? for a discussion).

The most general approach seems to be from the superfluid. This is quite appealing insofar as, unlikely the panoply of possible Mott states, the superfluid is unique, and has a symmetry which is independent of the boson filling. Thus the dual approach, based upon vortex degrees of freedom, generalizes directly to arbitrary filling factors. Moreover, we will see that the variety of distinct Mott states arises naturally from this description.

*) Strictly speaking, in the superfluid, the density is not exactly equal to \bar{n} , except when \bar{n} is an integer or half integer in the microscopic rotor model. What is important is not \bar{n} but the density f in the superfluid adjacent to the Mott state (within which f is independent of \bar{n} for a range of \bar{n} , it being incompressible). The actual value of \bar{n} should be adjusted to achieve $f = p/q$. We tacitly assume this is done below.

5.1. Vortex projective symmetry group

As for integral filling, we shift the dual vector potential to include the average dual flux, $A_{a\alpha} \rightarrow \bar{A}_{a\alpha} + A_{a\alpha}$, with

$$\bar{A}_{a2} = 2\pi f a_x, \quad \bar{A}_{a1} = 0, \quad (5.1)$$

corresponding to Landau gauge. Note that the specific gauge choice (and indeed *any* gauge choice) breaks naïve spatial lattice symmetries. Nevertheless, because $\epsilon_{\alpha\beta} \Delta_\alpha \bar{A}_{a\beta}$ represents a uniform gauge flux, this is an artifact of gauge fixing. Clearly, since $A_{a\alpha}$ is a dynamical variable, it is possible simply to undo the effect of any space group operation on $\bar{A}_{a\alpha}$ by an appropriate shift of $A_{a\alpha}$. Because the gauge-invariant flux is not changed by such an operation, this shift of $A_{a\alpha}$ must be pure gauge, i.e. a gradient $\Delta_\alpha \chi_a$, for some scalar χ_a . As a consequence, we can compose this shift with a pure gauge transformation – of both the vortex field θ_a (or equivalently ψ_a) and the gauge field – by the phase factor χ_a in order to undo the shift of $A_{a\alpha}$. By this reasoning, it is clear that for every operation in the space-group, there is a corresponding transformation consisting of a naïve space-group transformation *and* a gauge rotation of the vortex fields *without* any transformation of the gauge field. This transformation is almost unique, up to a global (i.e. a -independent) $U(1)$ phase rotation of the vortex fields. The global phase arbitrariness is allowed because a uniform gauge rotation has zero gradient and hence does not shift $A_{a\alpha}$.

In this way, by making some arbitrary phase choice for each group element, one associates a transformation with each operation in the space group. These new transformations generate some new group, which obeys the original group multiplication table *up to phase factors*, which in general cannot be removed. This is called a *projective representation* of the space group, and in a slight abuse of notation, we also call this new group a Projective Symmetry Group, or PSG. The proper subgroup (i.e. not including reflections) of the PSG on the square lattice is generated by the three operations associated with x and y translations, and a $\pi/2$ rotation (which we choose about a dual lattice site), which can be chosen as:

$$\begin{aligned} T_y &: \psi(a_x, a_y) \rightarrow \psi(a_x, a_y - 1) \\ T_x &: \psi(a_x, a_y) \rightarrow \psi(a_x - 1, a_y) \omega^{a_y} \\ R_{\pi/2}^{\text{dual}} &: \psi(a_x, a_y) \rightarrow \psi(a_y, -a_x) \omega^{a_x a_y}, \end{aligned} \quad (5.2)$$

with $\omega \equiv e^{2\pi i f}$. Specific algebraic relations follow from these definitions, notably

$$T_x T_y = \omega T_y T_x, \quad (5.3)$$

which informs us that, unlike in the original space group, the operations associated with translations in the PSG *do not commute*. The translational subgroup of the PSG is well-studied, and Eq. (5.3) is known as the magnetic translation algebra. The physical meaning of Eq. (5.3) is, as explained in the introduction, that the vortex acquires a dual Aharonov-Bohm phase of $2\pi f$ upon encircling a site of the direct lattice, containing on average f bosons.

The remaining algebraic relations between generators are unchanged from the original space group:

$$\begin{aligned} T_x R_{\pi/2}^{\text{dual}} &= R_{\pi/2}^{\text{dual}} T_y^{-1} \\ T_y R_{\pi/2}^{\text{dual}} &= R_{\pi/2}^{\text{dual}} T_x \\ \left(R_{\pi/2}^{\text{dual}}\right)^4 &= 1. \end{aligned} \tag{5.4}$$

5.2. Vortex multiplets

We again consider now the nature of the elementary vortex excitations, starting from Eq. (4.11). As in Sec. 4.3, at leading order in \tilde{t} , we must solve the tight-binding model arising from degenerate perturbation theory amongst the $|a\pm\rangle$ states, this time in the presence of the mean gauge field, Eq. (5.1). This is the Hofstadter problem, which is well-known generally to have a extremely complex “butterfly” spectrum.²⁴⁾ We are, fortunately, interested only in the lowest-energy states at the bottom of the lowest Hofstadter band. As for any particles, these must appear in multiplets comprising an irreducible representation of the symmetry group of the hamiltonian. In this case, this group is the PSG.

It is straightforward to see that, for a filling/dual flux with denominator $q > 1$, all representations of the PSG are *at least* q -dimensional. This follows because one may choose to, say, diagonalize T_y . However, by Eq. (5.3), acting with T_x on a state multiplies its eigenvalue of T_y by ω , hence this must be a linearly independent state to the initial one. This can be done repeatedly $q - 1$ times, until the q^{th} time, one arrives back at a state with the initial eigenvalue of T_y . Thus the PSG connects states of q different values of the quasimomentum. Since we used only Eq. (5.3), this conclusion is clearly true for the translational subgroup of the PSG alone, so representations of the full PSG can only be equal or larger.

It turns out, from explicit solution of the tight-binding model, that a q -dimensional irreducible representation (irrep) does exist for the full PSG, and moreover, this is the lowest energy vortex multiplet for the case of interest. Details of this construction can be found in Ref. 1). The result is that q vortex fields, φ_ℓ , $\ell = 0 \dots q - 1$ may be defined, as relativistic field operators (i.e. analogously to Eq. (3.9), as superpositions of “particle” (vortex) creation and “anti-particle” (anti-vortex) annihilation operators) for each member of the multiplet. Under translations,

$$\begin{aligned} T_x : \varphi_\ell &\rightarrow \varphi_{\ell+1} \\ T_y : \varphi_\ell &\rightarrow \varphi_\ell \omega^{-\ell}. \end{aligned} \tag{5.5}$$

Here, and henceforth, the arithmetic of all indices of the φ_ℓ fields is carried out modulo q , e.g. $\varphi_q \equiv \varphi_0$. Under the rotation,

$$R_{\pi/2}^{\text{dual}} : \varphi_\ell \rightarrow \frac{1}{\sqrt{q}} \sum_{m=0}^{q-1} \varphi_m \omega^{-m\ell}, \tag{5.6}$$

which is a Fourier transform in the space of the q fields. The full (improper) PSG is generated by including also reflections (defined here about x and y axes of the dual

lattice),

$$\begin{aligned} I_x^{\text{dual}} &: \varphi_\ell \rightarrow \varphi_\ell^* \\ I_y^{\text{dual}} &: \varphi_\ell \rightarrow \varphi_{-\ell}^* . \end{aligned} \quad (5.7)$$

A continuum field theory can be now constructed from the q -dimensional vortex multiplet. The effective action should be invariant under all the physical symmetries, with vortex fields transforming under the PSG and the dual $U(1)$ gauge symmetry. Restoring fluctuations of the gauge field, the critical action constructed in this manner, generalizing Eq. (4.14) to non-integer filling, has the form given in Eq. (1.2) in the introduction.

5.3. Order parameters

It is important to consider the observables in the problem. For integer filling, we discussed that φ is not itself a true “order parameter” because it is not gauge invariant. Physical quantities (e.g. superfluid density, compressibility, off-diagonal long-range-order) in that case are related just to properties of the dual gauge field. This is because local, gauge-invariant combinations of the single vortex field such as $|\varphi|^2$ etc. (related to the vortex/anti-vortex bound states discussed in Sec. 4.3.1) are scalars under all symmetries of the hamiltonian.

The situation is dramatically different for $q > 1$. While the above physical quantities are still related to properties of the dual gauge field, in general, gauge-invariant bilinears of the form $\varphi_\ell^* \varphi_{\ell'}$ are not scalars under the spatial symmetries. They can thus serve as order parameters for various types of symmetry breaking. Group theoretically, the direct product of an irrep of the PSG and its conjugate can be decomposed into a sum of true irreps of the ordinary space group (not projective representations). Happily, the basic components of these irreps can be constructed in generality.¹⁾ With the definition of Eq. (1.4) of the introduction, straightforward manipulations show that $\rho(\mathbf{Q})$ transforms exactly as expected for a Fourier component of a scalar “density” with wavevector \mathbf{Q} . Specifically, it is easy to verify that $\rho_{mn}^* = \rho_{-m,-n}$, and from Eqs. (5.5) and (5.6) that the space group operations act on ρ_{mn} just as expected for a density wave order parameter

$$\begin{aligned} T_x &: \rho_{mn} \rightarrow \omega^{-m} \rho_{mn} \\ T_y &: \rho_{mn} \rightarrow \omega^{-n} \rho_{mn} \\ R_{\pi/2}^{\text{dual}} &: \rho_{mn} \rightarrow \rho_{-n,m} . \end{aligned} \quad (5.8)$$

§6. Examples

While the set of different ρ_{mn} can describe a variety of different density wave orders in the Mott state, the number of such ordering patterns is limited, so the vortex theory actually constrains the nature of Mott insulating density ordering occurring in the neighborhood of a continuous transition to a superfluid. These orders can be determined from a mean-field analysis of the effective action \mathcal{S} , Eq. (4.14). We give examples for $q = 2, 3$. Further examples can be found in Ref. 1).

6.1. Half-filling and deconfined criticality

The case of $q = 2$, corresponding to bosons at half-filling, is particularly interesting. One has $\mathcal{L}_{\text{int}} = \mathcal{L}_4 + O(\varphi^6)$, with

$$\mathcal{L}_4 = \frac{\gamma_{00}}{4} (|\varphi_0|^2 + |\varphi_1|^2)^2 + \frac{\gamma_{01}}{4} (\varphi_0 \varphi_1^* - \varphi_0^* \varphi_1)^2. \quad (6.1)$$

It is convenient to make the change of variables

$$\begin{aligned} \varphi_0 &= \frac{\zeta_0 + \zeta_1}{\sqrt{2}} \\ \varphi_1 &= -i \frac{\zeta_0 - \zeta_1}{\sqrt{2}}. \end{aligned} \quad (6.2)$$

The action in Eq. (6.1) reduces to

$$\mathcal{L}_4 = \frac{\gamma_{00}}{4} (|\zeta_0|^2 + |\zeta_1|^2)^2 - \frac{\gamma_{01}}{4} (|\zeta_0|^2 - |\zeta_1|^2)^2. \quad (6.3)$$

The result in Eq. (6.3) is identical to that found in earlier studies^{15),16)} of the $q = 2$ case.

Minimizing the action implied by Eq. (6.3), it is evident that for $\gamma_{01} < 0$ there is a one parameter family of gauge-invariant solutions in which the relative phase of ζ_0 and ζ_1 remains undetermined. As shown in earlier work,¹⁵⁾ this phase is pinned at specific values only by an 8^{th} order term proportional to $\sim (\zeta_0 \zeta_1^*)^4 + \text{c.c.}$

The mean-field analysis finds three phases: First, phase (A): an ordinary charge density wave (CDW) at wavevector (π, π) . The other two states are VBS states in which all the sites of the direct lattice remain equivalent, and the VBS order appears in the (B) columnar dimer or (C) plaquette pattern. The phases (A), (B), and (C) appear in the upper-left, upper-right, and lower-right corner of the inset in Fig. 2. Note that the ‘‘site-centered stripe’’ phase in the lower-left of the inset, though it certainly can occur in lattice boson models, does not occur according to the vortex theory in the vicinity of the transition to the superfluid. The saddle point values of the fields associated with these states are:

$$\begin{aligned} (A) &: \zeta_0 \neq 0, \zeta_1 = 0 \text{ or } \zeta_0 = 0, \zeta_1 \neq 0. \\ (B) &: \zeta_0 = e^{in\pi/2} \zeta_1 \neq 0. \\ (C) &: \zeta_0 = e^{i(n+1/2)\pi/2} \zeta_1 \neq 0, \end{aligned} \quad (6.4)$$

where n is any integer.

6.1.1. Deconfined criticality

This particular example, for $\gamma_{01} < 0$, has recently been understood in much more detail. It turns out that this case, describing the transition from a superfluid to a columnar or plaquette VBS state, can be understood from a complementary point of view as a theory of *fractional* ‘‘half’’-boson excitations. It is too involved to fully explore this in detail in this paper, but we will at least uncover these fractional excitations in the dual theory.

For $\gamma_{01} < 0$, the mean-field solutions in the Mott state have both $\zeta_\ell = |\zeta|e^{i\vartheta_\ell}$, with $|\zeta|$ constant. Supposing slowly varying ϑ_ℓ , the effective phase-only action is

$$S_{eff} = \int d^2r d\tau \sum_\ell \frac{\rho'_s}{2} |\partial_\mu \vartheta_\ell - A_\mu|^2 + \frac{1}{2e^2} (\epsilon_{\mu\nu\lambda} \partial_\nu A_\lambda)^2, \quad (6.5)$$

with $\rho'_s = 2|\zeta|^2$. Consider a fixed ‘vortex’ (independent of τ) in one – say ϑ_0 – of the 2 phase fields, centered at the origin $r = 0$. One has the spatial gradient $\vec{\nabla} \vartheta_0 = \hat{\phi}/r$, while $\vec{\vartheta}_1 = 0$ (here $\hat{\phi} = (-y, x)/r$ is the tangential unit vector). Clearly, the action is minimized for tangential $\vec{A} = A\hat{\phi}$. Far from the ‘vortex’ core, the Maxwell term $(\epsilon_{\mu\nu\lambda} \partial_\nu A_\lambda)^2$ is negligible, so one need minimize only the first term in Eq. 6.5. The corresponding Lagrange density at a distance r from the origin is thus

$$\mathcal{L}'_v = \frac{\rho'_s}{2} [(1/r - A)^2 + A^2]. \quad (6.6)$$

Minimizing this over A , one finds $A = 1/(2r)$. Integrating this to find the flux gives

$$\oint \vec{A} \cdot d\vec{r} = \pi \quad (6.7)$$

Since the physical charge is just this dual flux divided by 2π , the ‘vortex’ in ζ_0 indeed carries fractional boson charge $1/2$.

Note that, because of the small 8^{th} order term locking the phases ϑ_0 and ϑ_1 together, such a ‘vortex’ in just one of these fields costs a divergent energy (actually linear in system size). This indicates these fractional particles are “confined” in the Mott state, like quarks in quantum chromodynamics. This confinement, however, becomes weaker and weaker as the SF-Mott QCP is approached, due to the smallness of the 8^{th} order term in this limit. In this sense – and in others discussed in Refs.¹⁹⁾ – this is a “deconfined QCP”.

A naïve extension of this argument would suggest the presence of charge $1/q$ for general q . It turns out that this generalization is not so simple, and while it can be made in some cases, there are considerable restrictions involved – see Ref. 1).

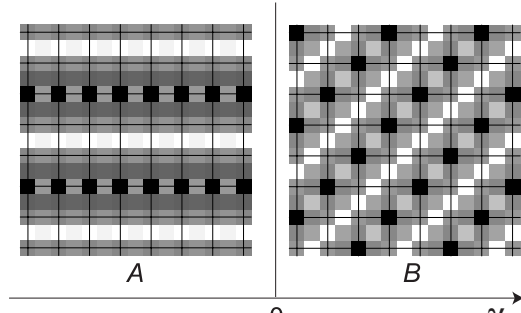
6.2. $q = 3$

Now there are 3 φ_ℓ fields, and the quartic potential in Eq. (6.1) is replaced by

$$\begin{aligned} \mathcal{L}_4 = & \frac{\gamma_{00}}{4} (|\varphi_0|^2 + |\varphi_1|^2 + |\varphi_2|^2)^2 \\ & + \frac{\gamma_{01}}{2} (\varphi_0^* \varphi_1^* \varphi_2^2 + \varphi_1^* \varphi_2^* \varphi_0^2 + \varphi_2^* \varphi_0^* \varphi_1 - \varphi_0^* \varphi_1^2 + \text{c.c.} \\ & - 2|\varphi_0|^2 |\varphi_1|^2 - 2|\varphi_1|^2 |\varphi_2|^2 - 2|\varphi_2|^2 |\varphi_0|^2). \end{aligned} \quad (6.8)$$

The results of a mean-field analysis for this potential are shown in Fig 3.

The states have stripe order, one along the diagonals, and the other along the principle axes of the square lattice.



Both states are 6-fold degenerate, and the characteristic saddle point values of the fields are

$$\begin{aligned}
 (A) : & \varphi_0 \neq 0, \varphi_1 = \varphi_2 = 0 \text{ or} \\
 & e^{i4n\pi/3}\varphi_2 = e^{i2n\pi/3}\varphi_1 = \varphi_0 \neq 0 \\
 (B) : & \varphi_0 = \varphi_1 = e^{\pm 2i\pi/3}\varphi_2 \\
 & \text{and permutations.}
 \end{aligned}
 \tag{6.9}$$

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