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Trapping centers at the superfluid–Mott-insulator criticality: Transition between charge-quantized states

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Under the conditions of superfluid–Mott-insulator criticality in two dimensions, the trapping centers—i.e., local potential wells and bumps—are generically characterized by an integer charge corresponding to the number of trapped particles (if positive) or holes (if negative). Varying the strength of the center leads to a transition between two competing ground states with charges differing by ± 1. The hallmark of the transition scenario is a splitting of the number density distortion $\delta n(r)$ into a half-integer core and a large halo carrying a complementary charge of $\pm\frac{1}{2}$. The sign of the halo changes across the transition and the radius of the halo r_0 diverges on the approach to the critical strength of the center, $V = V_c$, by the law $r_0 \propto |V - V_c|^{-\tilde{\nu}}$, with $\tilde{\nu} \approx 2.33(5)$.

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A two-dimensional (2D) system of bosons in a commensurate external potential/lattice in the regime of superfluid–Mott-insulator quantum criticality yields an example of nontrivial relativistic quantum field theory [1,2], which can be addressed experimentally with ultracold-atomic optical lattice emulators [3–7]. Among the fundamental problems of this theory is the question of the universal properties of polarons/impurities [8–12]. These properties fall into two rather different categories: transport properties and charge-quantization properties.

In the context of polaron physics, the notion of charge quantization emerges when there exist different states of a polaron characterized by an integer quantum number representing the number of particles of the medium bound to the impurity particle [13]. A necessary but not yet sufficient condition for polaron charge quantization to take place is the absence of broken $U(1)$ symmetry in the system of particles forming the medium.

In an incompressible medium, there exists a somewhat different and very transparent statement of the charge-quantization problem. Namely, the mobile impurity can be replaced with a static center, i.e., a short-ranged potential well/bump. Such a setup can be realized in ultracold-atomic experiments with single-site addressing techniques [14]. The charge of the center is then introduced as an integral of the number density variation created by the center. Inside the Mott insulator phase, the integer quantization of both the polaron and the center charges is quite obvious from the path-integral particle-hole representation of the bosonic ground state. In this case, the long-range density fluctuations are represented by a dilute gas of particle-hole loops, leaving no room for either a noninteger or an ill-defined charge. At the superfluid–Mott-insulator critical point in $d \geqslant 2$, where the compressibility is zero but the gap is absent, the question of charge quantization becomes quite subtle.

In this Rapid Communication, we address the question of the quantization of the charge of a center ξ in the superfluid–Mott-insulator quantum-critical ground state in 2D. With worm-algorithm path-integral Monte Carlo simulations [15] we find that ξ is generically an integer.

Consistent with the quantization of ξ, varying the strength of the center V leads to transitions between two competing values of the charge of the center, ξ_1 and $\xi_2 = (\xi_1 \pm 1)$. The transition turns out to be rather nontrivial. At the critical value $V = V_c$, the charge of the center is a *half integer*, $\xi = \xi_1 \pm \frac{1}{2}$. This peculiar state develops by the following critical scenario. When V is close enough to V_c, the integer total charge of the center comes with a specific bimodal density distribution: a half-integer core surrounded by a half-integer halo. The size of the halo r_0, playing the role of the healing length with respect to the total charge, diverges when $V \to V_c$,

$$r_0 \propto 1/|V - V_c|^{\tilde{\nu}}, \quad \tilde{\nu} = 2.33(5). \tag{1}$$

Across the transition point, the half-integer charge of the core remains intact while the charge of the halo changes its sign. The half-integer quantization of the halo charge—and, correspondingly the charge of the core—follows from the very fact of the existence of a halo with diverging size r_0. Indeed, the relativistic long-range physics of the $U(1)$ quantum criticality is particle-hole symmetric. Hence, there always exist two halo solutions that differ only by the sign of $\delta n(r)$, the density distortion. This implies that across the transition, the net charge of the center changes by (plus/minus) two times the absolute value of the halo charge. Given that the change of the center charge is ± 1, the halo charge then has to be $\pm\frac{1}{2}$.

In view of the divergent radius r_0 and scale invariance of the long-wave properties of our system, the structure of the halo has to be described by a universal scaling function f_{halo},

$$\delta n(r) = \pm r_0^{-2} f_{\text{halo}}(r/r_0) \quad (r \geqslant r_{\text{uv}}). \tag{2}$$

Here, r_{uv} is a certain ultraviolet cutoff. The form of the outer part of the halo,

$$f_{\text{halo}}(x) \propto \frac{1}{x^3} \quad \text{at } x \gg 1, \tag{3}$$

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has a rather simple physical nature. It corresponds to the universal asymptotic behavior of $\delta n(r)$ away from the center,

$$\delta n(r) \propto \chi(\mathbf{r}) \quad (r \to \infty), \tag{4}$$

dictated by the linear-response function

$$\chi(\mathbf{r}) = \int_0^\beta d\tau [\langle n(\mathbf{0},0) n(\mathbf{r},\tau)\rangle - |\langle n(\mathbf{0},0)\rangle|^2] \tag{5}$$

featuring the universal critical behavior

$$\chi(r) \propto \frac{1}{r^3} \quad [U(1) \text{ critical in 2D}]. \tag{6}$$

Equation (6) follows by the observation that upon the integration over $\mathbf{r}$ up to a certain macroscopic distance R, the right-hand side of (5) acquires the meaning of negative ground-state compressibility $-\kappa(R)$ for a subsystem of size $\sim R$. This quantity is known to scale as $\kappa(R) \propto R^{1-d}$ at the $U(1)$ critical point in d dimensions [2]. One thus arrives at (6) and also proves—using (4)—that in the linear-response limit, the charge of the center equals zero.

At $r \ll r_0$, the halo has a singular structure,

$$f_{\text{halo}}(x) \propto \frac{1}{x^s}, \quad s = 1 + 1/\tilde{\nu} \quad (x \ll 1). \tag{7}$$

Such a behavior is implied by (1). By continuity in r, the singular part of the V dependence of the expectation value of the center occupation number n_0 [to be specific about microscopic quantities, here we use the notation of the Bose-Hubbard model (8) that will be introduced below] should be consistent with Eq. (2) taken for a certain fixed microscopic value of $r \sim r_{\text{uv}}$ and V-dependent r_0. On the other hand, using the standard thermodynamic relation for the averaged partial derivative of the Hamiltonian, we have $n_0 = \partial E/\partial V$, where E is the ground-state energy. The singular part of the energy E_{sing} comes from the halo, and thus corresponds to the "half particle" delocalized over the radius $\sim r_0$. With the above-mentioned result for the finite-size compressibility, we have $E_{\text{sing}} \sim \kappa(r_0)$. This brings us to the relation (7) upon taking into account the scaling of r_0 with $|V - V_c|$, Eq. (1).

We simulate the standard Bose-Hubbard model on the square lattice [2], with the trapping center located at the site $i = 0$,

$$H = -\sum_{\langle ij\rangle} b_i^\dagger b_j + \frac{U}{2}\sum_i n_i(n_i - 1) - \mu \sum_i n_i + V n_0. \tag{8}$$

Here, $b_i^\dagger$ and b_i are, respectively, bosonic creation and annihilation operators on the site i; the symbol $\langle\cdots\rangle$ stands for nearest neighbors; U is the on-site interaction in units of hopping amplitude; the latter is set equal to unity. We work at the unit filling factor, setting U and the chemical potential μ equal to their critical values, $U_c = 16.7424(1)$, $\mu_c = 6.21(2)$ [16,17]. We use periodic boundary conditions, so that all the positions for the center are equivalent. The Hamiltonian (8) is directly relevant to optical lattice emulators [3].

To extract an accurate value of the universal critical exponent $\tilde{\nu}$, as well as to validate relation (7), we employ the three-dimensional (3D) classical J-current model [18] with $L^2 \times L_\tau$ sites,

$$H = \frac{1}{2K} \sum_{i,\hat{e}=\hat{x},\hat{y},\hat{\tau}}^{\Delta J=0} J_{i,i+\hat{e}}^2 - V \sum_{i_0=(\mathbf{0},\tau)} J_{i_0,i_0+\hat{\tau}}. \tag{9}$$

Here, $J_{i,i+\hat{e}}$ 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 $K_c = 0.333\,205(2)$.

Without loss of generality, we consider the repulsive case $V > 0$, so that the two competing ground states of the center have the charges $\xi_1 = 0$ and $\xi_2 = -1$. 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),

$$I(r) = \sum_{r_i \leqslant r} (n_i - 1). \tag{10}$$

For a system of 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,

$$\xi = I(\infty). \tag{11}$$

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

$$I(r) = \xi \pm \frac{\text{const}}{r} \quad (r \to \infty). \tag{12}$$

For a compelling demonstration of the quantization of ξ 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 $L \gg r_0$, Eq. (12) implies the following scaling ansatz,

$$I(r) - \xi = \pm L^{-1} f(r/L) \quad (r_0 \ll r \lesssim L), \tag{13}$$

where $f(x)$ is a certain scaling function such that $f(x) \propto 1/x$ at $x \ll 1$. An accurate calculation of ξ amounts then to checking the consistency of ansatz (13).

Apart from the finite-size effects there are also finite-temperature corrections. In our simulations, the temperature is adjusted to the system size by

$$T = c/L, \tag{14}$$

where c is the sound velocity, which is 4.8(2) for the Bose-Hubbard model [16] (for the J-current model, $c = 1$ in view of explicit symmetry between all 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.

In Fig. 1 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 a nonlinear response to take place at short distances. Consistency with the ansatz (13) confirms

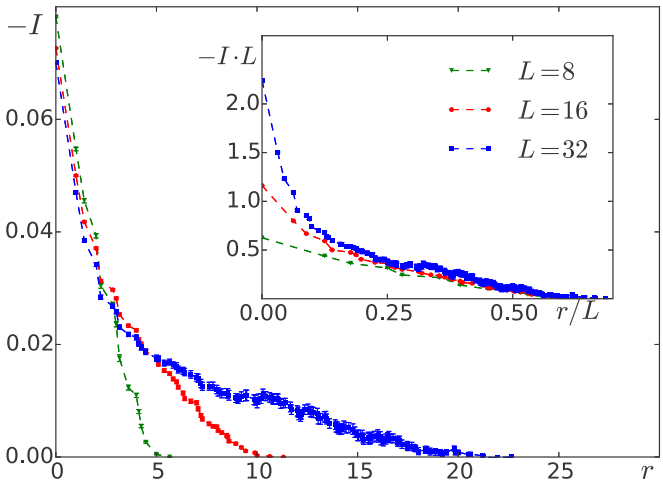

FIG. 1. The integral $I(r)$ at $V = 3.5$ and different system sizes L. The simulation is performed in the canonical ensemble with the total number of particles $N = L^2$. The inset shows consistency with the scaling ansatz (13) with $\xi = 0$, thus simultaneously verifying the linear-response asymptotic behavior (12) 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.

the linear-response asymptotic behavior (12) and demonstrates that $\xi = 0$ within our numeric resolution.

To accurately resolve universal features of the criticality of the transition between the $\xi = 0$ and $\xi = -1$ states, we resort to the J-current model in a (pseudo-)grand-canonical ensemble; see Fig. 2. In optical lattice emulators, a similar analysis can be performed if the role of the particle reservoir is played by the peripheral region of the system. In this case, the total number of particles is no longer a relevant observable. A way out is to deal with $I(r)$ at a certain large r. To model

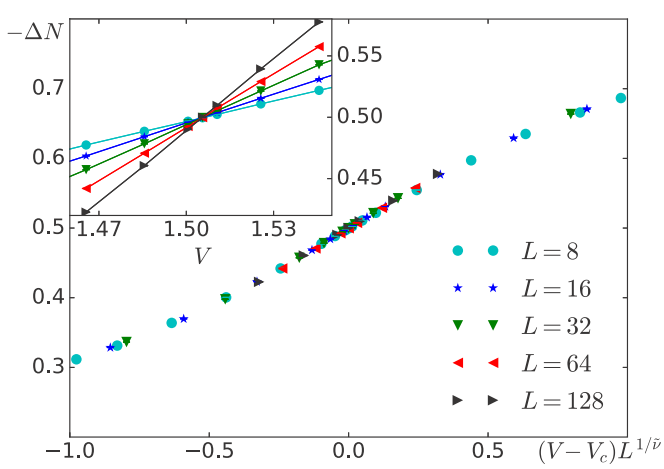

FIG. 2. The change in the total number of particles ΔN in the J-current model as a function of rescaled strength of the center at different system sizes L. The simulation is performed in the pseudo-grand-canonical ensemble containing only the two (most relevant) sectors of the total particle number, $N = L^2$ and $N = L^2 - 1$. Optimal fitting yields $V_c = 1.5056(5)$ and $\tilde{\nu} = 2.33(5)$. The inset shows bare (not scaled) data.

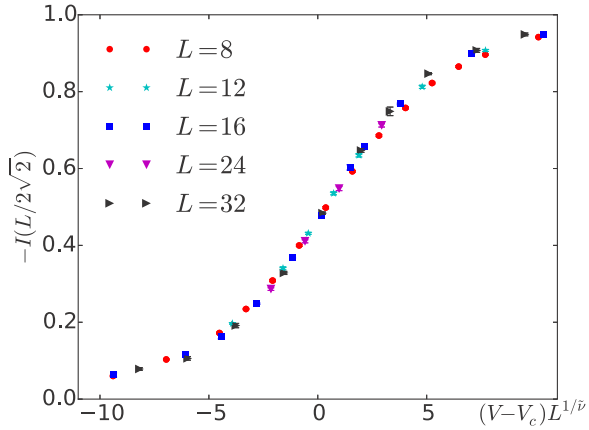

FIG. 3. The integral $I(L/2\sqrt{2})$ in the Hubbard model as a function of the rescaled strength of the center at different system sizes. The simulation is performed in the grand-canonical ensemble. The data are consistent with the scaling analysis of the transition in J-current model (see Fig. 2). The value $V_c = 6.86(8)$ is obtained from optimal fitting with $\tilde{\nu} = 2.33(5)$.

such a setup with the Hamiltonian (8), we take $r = L/2\sqrt{2}$ corresponding to one half of the largest possible r. The data presented in Fig. 3 are consistent with what we have learned from the J-current model.

A remark is in order here concerning the unambiguity of our conclusion about the nature of the transition. The temperature scaling (14) 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 ($\xi = 0$ and $\xi = -1$) 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. 4, we numerically validate the result (7) for the inner part of the halo. Integration of Eq. (7) over $\mathbf{r}$ leads to the scaling ansatz $I(r) = \xi_{\text{core}} \pm C_0(r/r_0)^{2-s}$, where ξ_{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, a 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 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. 4 demonstrate consistency with this scaling ansatz, with C_1 indistinguishable from $\frac{1}{2}$ within our numeric resolution.

Comparison to the Mott insulator case. To underline the specificity of the revealed charge-quantization properties of trapping centers at the superfluid–Mott-insulator criticality, it is very instructive to trace how these properties become qualitatively different upon entering the Mott insulator phase. In the latter case, the charge-quantization properties of trapping centers—identically the same arguments applying to polarons as well—are dictated by the following two circumstances:

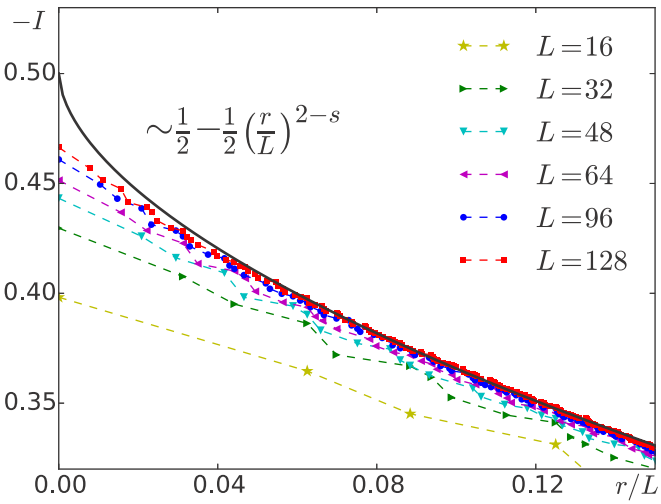

FIG. 4. Revealing the singularity of the inner part of the halo with the J-current model simulated at the critical point in the canonical ensemble $N = L^2$. The dashed lines are only to guide the eye. In the macroscopic limit and at $r/L \ll 1$, the curves saturate to the law $I(r) + \frac{1}{2} = C_1(r/L)^{2-s}$. The solid line represents this law with $s = 1.43$ and $C_1 = \frac{1}{2}$.

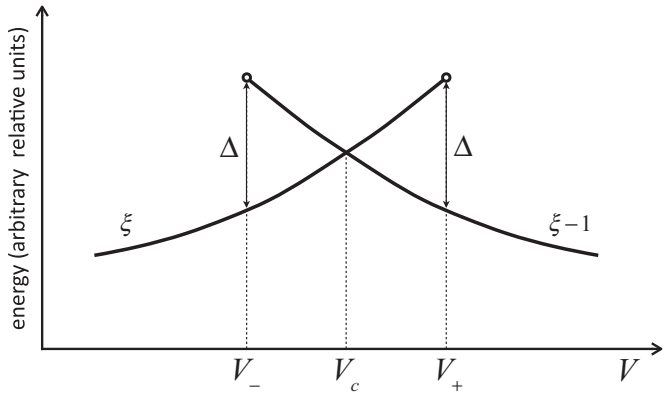

FIG. 5. Schematic behavior of the trapping center in the Mott insulator phase: The ground-state energies, as functions of the center strength V, for two competing ground states. The value V_c corresponds to a nominal transition between the state of the charge ξ and the state of the charge $(\xi - 1)$. The values V_- and V_+ are the two end points defined by the condition that the energy difference between the two competing states is exactly equal to the insulating gap Δ.

(i) the presence of a finite insulating gap and (ii) the existence of well-defined particle/hole elementary excitations with parabolic dispersion in the long-wave limit. The finite insulating gap immediately guarantees the integer quantization of the center charge in any dimension. Furthermore, the notion of the transition between the ground states of different center charges becomes merely nominal. As long as the energy difference between the two states does not exceed the gap, a decay of one into another (assisted by particle/hole emission) is kinematically forbidden. In the vicinity of the "transition" point V_c, we thus have two stable ground states, each in its own charge sector. While (in the Mott insulator phase) no physical transition occurs at V_c in the Mott insulator phase, a new type of critical point appears, namely, the end point. For each transition point V_c, there are two associated end points, $V_+ > V_c$ and $V_- < V_c$; see Fig. 5. If the transition at V_c is between the state with the center charge ξ (at $V < V_c$) and the state with the center charge $(\xi - 1)$ (at $V > V_c$), then V_- is the lower end point for the state with the center charge $(\xi - 1)$ and V_+ is the upper end point for the state with the center charge ξ. Correspondingly, in the interval $[V_-, V_+]$, both ξ and $(\xi - 1)$ are legitimate values of the center charge. When V approaches the end point V_+ from below, the charge-ξ center experiences a dramatic evolution towards a loose dimer consisting of a well-localized charge-$(\xi - 1)$ center and a weakly bound particle. At the end point V_+, the particle unbinds. A similar picture, up to interchanging $\xi \leftrightarrow (\xi - 1)$ and replacing the weakly bound particle with a weakly bound hole, takes place when V approaches the end point V_- from above.

The above-discussed loose-dimer scenario of the end point rests heavily on the parabolic—as opposed to linear at criticality—dispersion relation of particles/holes. This explains why this scenario does not apply to the superfluid–Mott-insulator criticality. In the latter case, in 2D, we do have a loosely bound object—the halo—when V approaches V_c. Nevertheless, the half-integer charged halo weakly bound to a half-integer charged center involves a qualitatively different critical physics.

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