Weak First-Order Superfluid-Solid Quantum Phase Transitions

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We study superfluid–solid zero-temperature transitions in two-dimensional lattice boson/spin models by Worm-Algorithm Monte Carlo simulations. We observe that such transitions are typically first-order with the exception of special high-symmetry points which require fine tuning in the Hamiltonian parameter space. We present evidence that the superfluid–checkerboard solid and superfluid–valence-bond solid transitions at half-integer filling factor are extremely weak first-order transitions and in small systems they may be confused with continuous or high-symmetry points.

Recently, there has been an increased interest in superfluid–solid (SF-S) quantum phase transitions in lattice boson/spin systems [1, 2, 3, 4]. [By 'solid' we mean an insulating state featuring the broken translation symmetry—like checkerboard solid/antiferromagnet (CB) or valence bond solid (VBS), as opposed to the Mott insulator which preserves the translation symmetry.] On one hand, this interest is stimulated by experimental perspectives of studying such transitions in optical lattices [3], on the other hand, the SF–VBS transition in a $(2 + 1)$-dimensional system has been argued to be the simplest example of qualitatively new type of quantum criticality, that does not fit the standard Landau-Ginzburg-Wilson paradigm [4]. Intriguing data on the SF-S transitions were obtained by direct Monte Carlo simulations of quantum systems [1, 2]. It was observed [1] that the SF-CB transition in the hard-core bosonic model with nearest- and next-nearest-neighbor interaction remains remarkably insensitive to the explicit Heisenberg symmetry breaking. The transition is numerically indistinguishable from that of the Heisenberg spin-1/2 model: a degenerate (hysteresisless) transition. In simulations of the 2D quantum XY model with ring exchange [2], the SF-VBS transition was interpreted as the second-order one, which suggested its understanding in terms of the deconfined quantum critical point [4].

In this Letter, we perform a careful finite-size analysis of the SF-CB and SF-VBS transitions by simulating a generalized (2+1)-dimensional J-current model [5], which is a discrete-imaginary-time analog of the quantum boson/spin lattice system. The simplicity and flexibility of our model in combination with the efficient Worm Algorithm allow us to arrive at a definitive conclusion that in SF-CB and SF-VBS cases we are dealing with anomalously weak first-order phase transitions. Moreover, the two transitions are remarkably similar to each other. In both cases, small enough critical systems mimic the behavior of a highly symmetric model with broken symmetry. The SF-CB case corresponds to the O(3)-symmetry of the Heisenberg model, while in the SF-VBS case we clearly see a quasi-O(4) behavior that manifests itself as a coexistence at the critical point of the superfluid response and both (x- and y-) VBS orders, in arbitrary proportions.

We confine ourselves to the case when the statistics of (2+1)-dimensional particle trajectories in imaginary time (worldline configurations) is positive definite. What groundstates can emerge under this condition? The state with chaotic (unstructured) typical worldline configuration is SF. Indeed, the absence of structure implies fluctuations of the worldline winding numbers, W, and thus a finite superfluid response which is given by the mean square of W [6], see Eq. (4) below. [One can hardly extend this argument to cases when the configuration weight is not positive definite, since the notion of a typical configuration becomes vague.] In SF, the U(1) symmetry is broken (at least in a topological sense). The only way to restore this symmetry is to suppress fluctuations of W which seems to be impossible without structuring worldline configurations in such a way that for each imaginary-time moment the position of each worldline in the corresponding real-space plane can be unambiguously associated at the microscopic level with one of the lattice sites/bonds, and vice versa. If the total number of the worldlines is not equal to a multiple of the number of sites/bonds, the structured worldline configuration immediately implies a broken translation symmetry. This consideration leads to the conjecture that for models with the positive definite statistics of worldline configurations and non-integer filling factor the generic groundstate should feature an order, either SF or solid, or both (supersolid). Groundstates with none symmetry being broken ("quantum disorder") may then occur only as critical points separating the ordered states.

In the path-integral representation, we see no qualitative difference between the site- and bond-based solids since both are characterized by the worldline structuring, in the above-mentioned sense. In either case, zero-point fluctuations necessarily include *permutations* of two and more lines, and thus on large scales such microscopic details as the most probable positioning—on sites or on bonds—of the worldlines can hardly be relevant to the universal properties of the SF–S transition. The only property that seem to be crucial is the symmetry of the emerging lattice.

In terms of algorithmic simplicity and numerical ef-

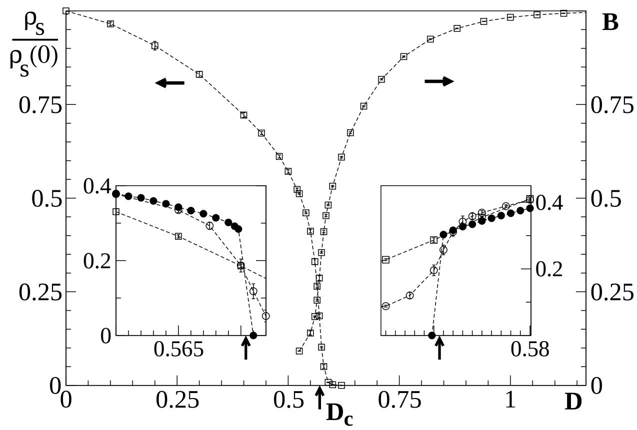

FIG. 1: SF stiffness ρ_s and VBS order parameter B dependence on the coupling strength D for $L = 16$ (squares), $L = 32$ (open circles on inset) and $L = 64$ (filled circles on inset) systems. A closer look at the transition point is provided in the insets. Error bars are shown for all points (in some cases these are smaller than the symbol size).

ficiency, classical $(d + 1)$-dimensional analogs of d-dimensional quantum systems offer a significant advantage. This approach was successfully used previously in the studies of disordered [5, 7, 8] and two-component systems [9]. In addition, classical models offer more freedom in "designing" effective models with complex phase diagrams. The so-called J-current model of Ref. [5] is obtained by considering trajectories in discrete imaginary time. Let $\mathbf{n} = (\mathbf{x}, \tau)$ denote points of the $(d + 1)$-dimensional space-time lattice, and integer currents $J_\nu(\mathbf{n})$ with $\nu = \hat{x}, \hat{y}, \hat{\tau}$ specify how many particles are going from site $\mathbf{n}$ in direction ν. In this language, currents in the time-direction represent occupation numbers, and currents in the space directions represent hopping events. The continuity of trajectories requires that $\sum_\nu [J_\nu(\mathbf{n}) - J_\nu(\mathbf{n} - \nu)] \equiv 0$.

The simplest J-current model at half-integer filling factor is obtained by writing the potential energy term in the particle-hole symmetric form

$$S_J = 2J \sum_{\mathbf{n}, \nu \neq \hat{\tau}} \left(J_{\hat{\tau}}(\mathbf{n}) - \frac{1}{2} \right) \left(J_{\hat{\tau}}(\mathbf{n} + \nu) - \frac{1}{2} \right) , \quad (1)$$

and restricting currents along $\hat{\tau}$-bonds to take on just two values, 0 and 1. The kinetic energy term is simply

$$S_K = K \sum_{\mathbf{n}, \nu \neq \hat{\tau}} |J_\nu(\mathbf{n})| , \quad (2)$$

with the restriction that allowed values for spatial currents are 1, 0, and -1 values. To exclude somewhat pathological cases with two hopping events happening at the same space-time point, we further require that $\sum_{\nu \neq \hat{\tau}} |J_\nu(\mathbf{n})| + |J_\nu(\mathbf{n} - \nu)| \leq 1$. Finally, we introduce interactions between the spatial currents on n.n. bonds which favor VBS

$$S_D = -D \sum_{\mathbf{n}, \nu \neq \hat{\tau}} |J_\nu(\mathbf{n})| \sum_{\mu \neq \nu} (|J_\nu(\mathbf{n} + \mu)| + |J_\nu(\mathbf{n} - \mu)|) . \quad (3)$$

Equal-time coupling ($\mu \neq \hat{\tau}$) favors simultaneous hopping events of particles on the same plaquette and is reminiscent of the ring exchange term in quantum models [2]. Phonon mediated exchange is another known mechanism of dimerization in spin Pierles systems [10], and in Eq. (3) it is represented by coupling between bonds connecting the same sites and shifted in the time direction. With all three terms combined, $S = S_J + S_K + S_D$, the resulting model has SF, CB, and VBS states in its phase diagram.

First we study the SF-VBS transition along the $J = 0$, $K = 0.4$ line. Superfluid stiffness is determined by the statistics of winding number fluctuations [6]

$$\rho_s = \langle W^2 \rangle / 2L , \quad (4)$$

and the VBS order parameter is characterized by the staggered distribution of spatial currents along $\hat{x}$ and $\hat{y}$ directions

$$B_\nu = L^{-(d+1)} \sum_{\mathbf{n}} |J_\nu(\mathbf{n})| \, e^{i\mathbf{n}\mathbf{q}} , \quad (5)$$

where $\nu = \hat{x}$ and $\nu = \hat{y}$ for $\mathbf{q} = (\pi, 0, 0)$ and $\mathbf{q} = (0, \pi, 0)$, respectively. We find it convenient to introduce a single VBS order parameter with positive definite estimator which takes on finite value $\sim \mathcal{O}(1)$ in the VBS phase, $B = |B_{\hat{x}}| + |B_{\hat{y}}|$. For completeness, we also define here the CB order parameter as

$$M_\tau(\mathbf{q} = (\pi, \pi, 0)) = L^{-(d+1)} \sum_{\mathbf{n}} J_{\hat{\tau}}(\mathbf{n}) e^{i\mathbf{n}\mathbf{q}} . \quad (6)$$

and $M = |M_\tau|$.

In Fig. 1 we show rescaled data for the SF stiffness $\rho_s / \rho_s(D = 0)$ and VBS order parameter. The main plot for $L = 16$ demonstrates strong suppression of ρ_s and B near the critical point [$D_c \approx 0.5705(2)$] which is typical for continuous phase transitions. Similar behavior was reported previously for the ring-exchange model in Ref. [2]. However, in the insets we clearly see that finite-size scaling is incompatible with the second-order transition scenario—the curves $\rho_s(D)$ for different sizes L intersect each other without any further rescaling indicating that large systems are more ordered in the vicinity of the critical point. Similar behavior is observed for the curves $B(D)$. The most obvious scenario is then a first-order transition where the intersection of finite-size curves at the critical point is allowed. Apparently, the transition is *weakly* first-order because (i) both order parameters are strongly suppressed at D_c, and (ii) simulations for $L^3 = 32^3$ system do not show any hysteresis, though the autocorrelation time is very long at D_c.

The other surprising fact is that the region where ρ_s for $L = 16$ is below the corresponding curves for $L = 32$ and $L = 64$ is rather extended, while in first-order transitions

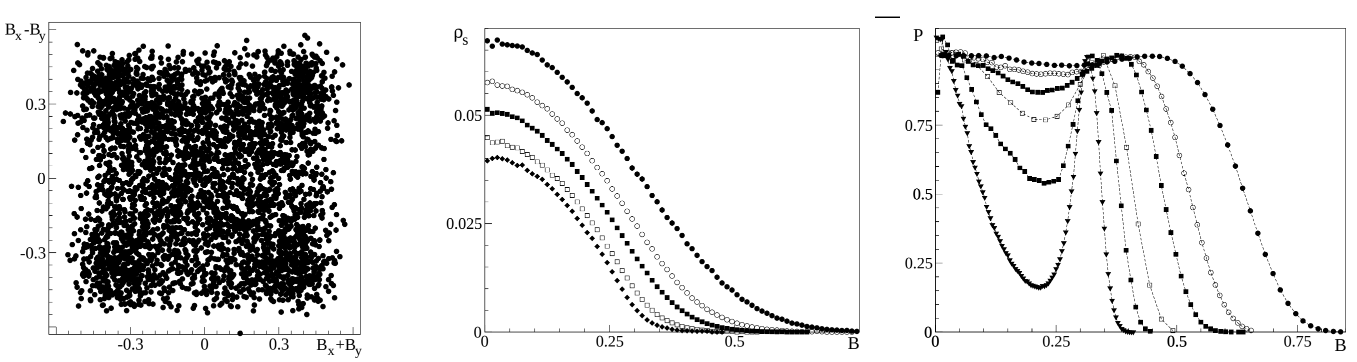

FIG. 2: Statistics of fluctuating SF and VBS order parameters. Left panel: points of the "black square" are obtained for MC configurations separated by equal long time intervals for $L = 16$ and $D = 0.5727$. Middle panel: SF stiffness is calculated as a function of B for various system sizes. From top to bottom curves are plotted at corresponding finite-L "transition points" (see the text), for ($L = 8,\ D = 0.5742$), ($L = 12,\ D = 0.5738$), ($L = 16,\ D = 0.5727$), ($L = 24,\ D = 0.5715$), ($L = 32,\ D = 0.5712$), ($L = 48,\ D = 0.5705$). Right panel: the coarse-grained distribution of the average density of points in the $B_{\hat{x}}, B_{\hat{y}}$-square along the $B = |B_{\hat{x}}| + |B_{\hat{y}}|$=const lines for the same set of system sizes and values of D as in the middle panel.

it is expected to be macroscopically small. It appears as if the superfluid order parameter Ψ experiences anomalously large fluctuations in small systems. To explain it we first speculate (and later prove numerically) that in the vicinity of the critical point the system is best described by the four-dimensional order parameter, $\vec{S}$, and the O(4)-symmetry is broken at D_c . Formally, $B_{\hat{x}}$, $B_{\hat{y}}$ and two components of Ψ represent observable (linearly independent) projections of $\vec{S}$; correspondingly, in the $(B_{\hat{x}}, B_{\hat{y}}, \Psi)$-space the O(4)-sphere is seen as a four-dimensional surface with the sphere topology. In this scenario, if the O(4)-symmetry is exact then any value of $\vec{S}$ is equally probable at D_c, i.e. solid orders along both spatial direction and superfluidity may coexist.

An analogous well-known example of the O(3)-symmetric point is provided by the SF-CB transition in the 2D quantum XXZ-antiferromagnet with n.n. exchange interactions. In this case, the XY order parameter $S_x + iS_y \equiv \Psi$ and the CB order parameter $S_z \equiv M$ form a three-dimensional vector $\vec{S}$. The critical point itself is described by the SU(2)-symmetric Heisenberg Hamiltonian. Since the O(3)-symmetry is spontaneously broken in the ground state of the Heisenberg model, at the transition both ρ_s and M change discontinuously in the thermodynamic limit, but this change occurs without energy barriers and is preceded by anomalously large fluctuations and long autocorrelation times in finite systems.

If the outlined picture is correct, then small perturbations which explicitly break the O(n) symmetry at the *microscopic* level should result in generic weak first-order transitions. Indeed, in the spontaneously ordered state all renormalizations are finite. Thus symmetry breaking perturbations, which couple to the *long-range* order, result in the non-flat macroscopic energy/effective action

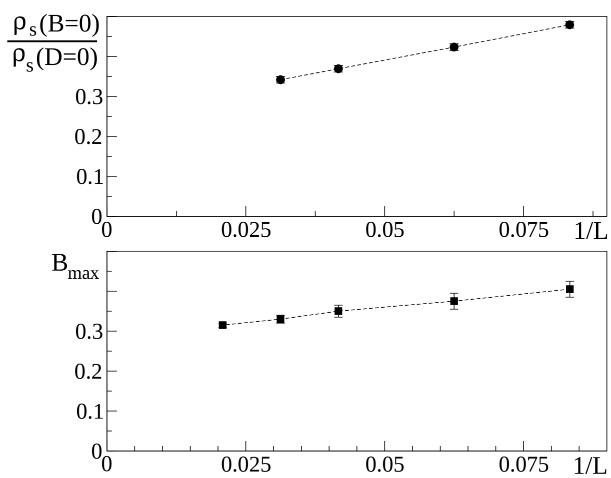

FIG. 3: System size dependence of $\rho_s(B = 0)/\rho_s(D = 0)$ (circles) and $B_{\max}$ (squares) from Fig. 1.

profile for the order parameter. Phase transitions are, then, between energy minima separated by macroscopic barriers which may, however, remain relatively weak in small systems. The J-current model studied here has no microscopic symmetries mandating exact O(4)- or O(3)-symmetry of the critical point. We conclude then that SF-VBS and SF-CB transitions are expected to be first order, and in the rest of the paper we present evidence that this is indeed so.

First, we demonstrate that relatively "small" (hundreds of particles!) systems in the vicinity of the critical point behave as if $(B_{\hat{x}}, B_{\hat{y}}, \Psi)$ fluctuations are confined to some surface, not volume, and it is not possible to have all three order parameters fluctuating to zero. In the left panel of Fig. 2 we show statistical fluctuations of the

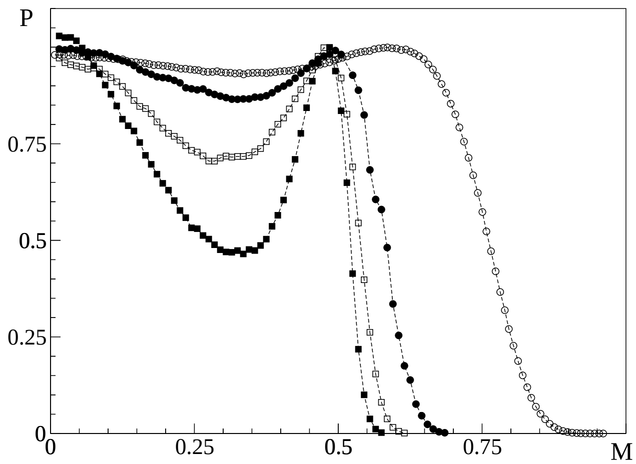

FIG. 4: The coarse-grained distribution of the CB order parameter for various system sizes; from right to left: ($L = 8,\ J = 0.450$), ($L = 16,\ J = 0.4205$), ($L = 24,\ J = 0.4189$), ($L = 32,\ J = 0.4186$).

VBS order parameters for $L = 16$ and $D = 0.5727$. The density of points in the $B_{\hat{x}}, B_{\hat{y}}$ "black square" is nearly homogeneous, i.e. the system is equally likely to be found with small or relatively large VBS order oriented at any angle relative to $\hat{x}, \hat{y}$-directions. Moreover, the boundary shape suggests that $B_{\hat{x}}$ and $B_{\hat{y}}$ fluctuations happen on the $B = f(|\Psi|)$ surface. The middle panel of Fig. 2 shows that indeed the values of B and ρ_s are strongly correlated [$\rho_s(B)$ is defined as the average, see Eq. (4), over configurations with the VBS order parameter $\in (B-\delta, B+\delta)$]. We see that, ρ_s is largest when $B \to 0$, i.e. despite large fluctuations of all order parameters, they never vanish simultaneously.

Finally, in the right panel we plot the average density of points in the $B_{\hat{x}}, B_{\hat{y}}$-plane along the B=const cuts for various system sizes. In each case, we adjusted the coupling constant D so that the distribution function $P(B)$ is "maximally flat", or the two maxima are at equal heights. Normalization was set to have the large-B maximum equal unity. The density profiles are nearly flat for $L = 6, 12, 16$ though with a tiny minimum between the VBS and SF regions. It appears as if physical order parameters belong to some four dimensional surface and may diffuse over it without large effective action barriers.

The minimum gets more pronounced for $L = 24, 32$, and breaks the distribution into well separated peaks for $L > 48$, i.e. the energy barrier finally gets large enough to localize the order parameter in one of the phases. The two-peak structure is a smoking gun evidence that the transition is ultimately weak first-order. Further evidence is provided by finite-size scaling of the critical-point distribution functions, i.e the dependence of $\rho_s(B = 0, L)$ (normalized to $\rho_s(D = 0)$ as in Fig. 1) and the position of the $P(B)$ distribution maximum, $B_{\max}(L)$. The data in Fig. 3 suggest that both quantities saturate to finite values in the thermodynamic limit.

The study of the SF-CB transition along the $K = 0.7$, $D = 0$ line reveals a remarkable similarity with the SF-VBS point. At $J_c = 0.4184(2)$ the superfluid and solid orders exchange places with pronounced fluctuations of both order parameters in small systems. These fluctuations are almost identical to what is expected for the O(3)-symmetric Heisenberg point where the distribution function for the staggered order parameter, $P(M < M_{\max}) = P(S_z)$ is a step function. However, in larger systems a minimum in $P(M)$ is developed. The double-peak structure of $P(M)$ for $L = 32$ leaves no doubt that we are actually dealing with the weak first-order transition. Apparently, system sizes in the study of the SF-CB point in Ref. [1] were too small to see the first-order transition.

At certain conditions (which with J-current model can be easily achieved by adding appropriate terms) the supersolid (SS) phase may intervene between SF and S phases. In this case, the vicinity to a (quasi-)O(3)/O(4) symmetric point with broken symmetry may render the SF-SS and SS-S transitions also first order, while normally one might expect them to be of the second order.

In conclusion, we note that weak first-order transitions discussed here can hardly be an artifact of the J-current model since they reveal themselves on large space-time scales.

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