# Two-dimensional superfluidity and localization in the hard-core boson model: A quantum Monte Carlo study

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Quantum Monte Carlo simulations are used to investigate the two-dimensional superfluid properties of the hard-core boson model, which show a strong dependence on particle density and disorder. We obtain further evidence that a half-filled clean system becomes superfluid via a finite-temperature Kosterlitz-Thouless transition. The relationship between low-temperature superfluid density and particle density is symmetric and appears parabolic about the half-filling point. Disorder appears to break the superfluid phase up into two distinct localized states, depending on the particle density. We find that these results strongly correlate with the results of several experiments on high-$T_c$ superconductors.

Quantum systems of interacting bosons in clean or disordered media have been used to study a variety of interesting problems, including the superfluidity of $^4$He, superconductor-insulator transitions in thin films, and vortex dynamics in type-II superconductors. Recently, the relation between superconducting transition temperature ($T_c$) and carrier density ($\delta$) in various copper-oxide superconductors was found to obey a universal bell-shape curve.[1–3] This finding also shows that the superfluid-like condensation of charged bosons (local Cooper pairs) is crucial for high-$T_c$ superconductivity, based on some common features of copper oxides: the extremely short coherence length implying pointlike Cooper pairs, and the layered structure which confines the carriers mainly to two-dimensional (2D) $CuO_2$ layers. From the analysis of muon-spin-relaxation ($\mu$SR) and transport measurements, Schneider and Keller[2] argued that such condensation of extreme type-II superconductors belongs to the classical $XY$ universality class in three dimensions, and Zhang and Sato[3] surmized that the bosons involved are actually bipolarons. In this model, Cooper-pair bosons whose binding energy is much larger than condensation energy are assumed to exist below $T_c$(onset), and superconductivity appears via the phase coherence of preexisting bosons.

Here, within the boson framework, we propose a quantum $XY$ universality class in two dimensions. We examine a 2D lattice boson Hubbard model[4] specified by hard-core repulsive interactions and random potentials. The phase diagram depends on the temperature, particle density, and also on the degree of disorder. First and foremost, when the particle density is varied, the phase diagram should be perfectly symmetric about the half-filling level, because of the particle-hole symmetry. Second, the hard-core Bose gas has mathematical analogy to the quantum spin problem.[5] From previous studies of a spin-1/2 $XY$ model,[6–9] one may expect that, for a clean boson system, the Kosterlitz-Thouless (KT) transition[10] takes place and 2D superfluidity arises below a finite critical temperature $T_{\rm KT}$. Also, regarding different bosonic systems, there are early numerical works suggesting a KT transition in a Coulomb gas model[11] and in a soft-core model.[12] Third, at sufficiently strong disorder, dense Bose gas is expected to exhibit a localized phase called the Bose glass.[4,13] Through a quantum Monte Carlo (MC) simulation, this paper provides further support for the superfluid KT transition of the hard-core boson model in the half-filling case, and sheds light on density-modulation and localization effects in 2D superfluidity. Our simulation results strongly correlate with recent experimental data in copper-oxide superconductors, including the $T_c$ vs $\delta$ relationship and the nature of superconducting phase transition.

The Hamiltonian of hard-core bosons is expressed as

$$H_{\rm boson} = -\frac{t}{2}\sum_{\langle i,j\rangle}(a_i^\dagger a_j + a_j^\dagger a_i) + \sum_{i=1}^{N} v_i n_i + H_{\rm HC} \quad (1)$$

for a square lattice of size $L\times L$. Here the first sum is the kinetic energy of bosons, where the hopping constant $t=\hbar^2/2m_b^* a^2$ with effective mass $m_b^*$ and lattice spacing $a$. The second part represents the potential energy from on-site disorders with a uniform distribution $v \in [-\Delta,\Delta]$. The hard-core interaction $H_{\rm HC}$ inhibits the double occupancy of bosons at each site. This interacting Bose gas can be transformed into an equivalent spin-1/2 $XY$ system in a randomly varying magnetic field, such that $H_{\rm boson} \rightarrow H_{\rm spin} = -t\sum_{\langle i,j\rangle}(S_i^x S_j^x + S_i^y S_j^y) + \sum_i v_i S_i^z$, by setting $a^\dagger = S^x + iS^y$, $a = S^x - iS^y$, and $n = S^z + 1/2$ with the spin-1/2 operator $\mathbf{S} = (S^x, S^y, S^z)$.[5]

To simulate the equilibrium state of such a quantum system efficiently, we use the path-integral approach based on the Suzuki-Trotter transformation.[7,8] The 2D bosonic system (under periodic boundary conditions) is transformed to a 3D (torus with space and imaginary-time dimensions) classical system of boson world lines. Possible paths of the world lines are topologically characterized by particle number and winding number, where the winding number ($W$) is defined by counting how many times the world lines wind around the torus in space directions. For the microcanonical ensemble of bosons (fixed particle density $n_b$), we carried out MC sampling of the world lines, by utilizing an algorithm

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previously developed for the spin model. ( See Ref. 7 for details of the simulation method, and Ref. 14 for some technical remarks, respectively.) The superfluid density $n_s$ corresponds to the free energy change due to twisting the phase of order parameter along one lattice boundary, and this quantity can be computed directly from winding number fluctuations

$$n_s = (k_B T/t)\langle W^2 \rangle \tag{2}$$

in the path-integral representation.[15] For the MC sampling, together with conventional local moves of world lines, we also made global update of winding number $W$,[11,12] such that all the transitions to different values of $W$ are allowed. In contrast, most previous spin simulations[6,9] were limited to a fixed condition of $W = 0$ while the particle number was variable. Since the present $W$-variable algorithm is ergodic regarding winding number, we can evaluate $n_s$ exactly for a finite-size lattice. This computational approach is complementary to earlier quantum MC studies[6,9] and exact diagonalization study[13] on the similar model.

Figure 1 shows the numerical results of a clean half-filled system ($\Delta = 0$, $n_b = 1/2$) with different size lattices ($L = 4, 6, 8$). The temperature dependence of 2D superfluid density is shown in Fig. 1(a). For $T < T_{\rm KT} = 0.40(5)\, t/k_B$, $n_s(T)$ grows remarkably and becomes almost independent of the lattice size, while, for $T > T_{\rm KT}$, it is suppressed with increasing size. At low temperatures, $n_s$ reaches 0.27(1) for the $L = 8$ lattice, compared to 0.28 given by the exact diagonalization of the much smaller ($L = 4$) lattice.[13] Thus, even at the ground state, the superfluid fraction is at most $n_s/n_b \approx 0.54$ in the thermodynamic limit, and the normal-fluid component remains large. This indicates a strong renormalization effect due to quantum fluctuations, while the thermal fluctuations cause the vortex-antivortex pairs to unbind at high temperatures. The value of $T_{\rm KT}$ is quite consistent with the KT universal jump condition, which satisfies $n_s(T_{\rm KT}) = 2k_B T_{\rm KT}/\pi t$ denoted as a dotted line in Fig. 1(a). Moreover, to get a clearer sign of the KT transition, we calculated the temperature derivative of $n_s$ using the fluctuation formula

$$\partial(\beta n_s)/\partial\beta = \langle W^2 \rangle \langle E \rangle - \langle W^2 E \rangle, \tag{3}$$

where $E$ is the total energy and $\beta = 1/k_B T$. As seen in Fig. 1(c), the peak value of $\partial(\beta n_s)/\partial\beta$ grows rapidly near $T = T_{\rm KT}$, as the lattice size increases. In sufficiently large lattices, Eq. (3) reduces to the energy difference $\Delta E$ between periodic and antiperiodic boundary conditions. It should be noted that, for the classical $XY$ model, an analogously divergent sign of $\Delta E$ was used as a decisive evidence for the KT transition.[16] On the other hand, the peak value of specific heat tends to saturate at $C_v = 0.62(1)$ just above $T_{\rm KT}$ with the increase in size, as shown in Fig. 1(c). Although it is well known that free Bose gas in two dimensions never condenses at finite temperatures, these numerical observations definitely support the view that the *hard-core* nature of interactions between bosons leads to the superfluid phase through the finite-temperature KT transition, while the quantum fluctuations are rather significant at low temperatures.

Figure 2 shows how the superfluid density depends on the Bose particle density and the degree of disorder ($\Delta$), at low temperature $T = 0.25\, t/k_B$. Note that the relationship between the superfluid density $n_s$ and the doping density $n_b$ is approximated well, although not exactly, by the parabolic form $n_s \propto (n_b - n_0)(1 - n_b - n_0)$ with some constant $n_0$. Here $n_0 = 0.06$, 0.13, 0.13, and 0.15 for various degrees of disorder $\Delta = 0$, 1.0, 1.25, and 1.75, respectively. In comparison, in a one-dimensional (1D) pure system, the exact result $n_s = \sin(\pi n_b)/\pi$ is obtained.[17] The symmetry about half filling is rigorous in both clean and disordered systems, since the model involves the particle-hole symmetry due to hard-core interactions. In the presence of disorder the parabola seems to be preserved, and in addition the onset of superfluidity can be found at a common value of $n_0 \approx 0.1$, despite large

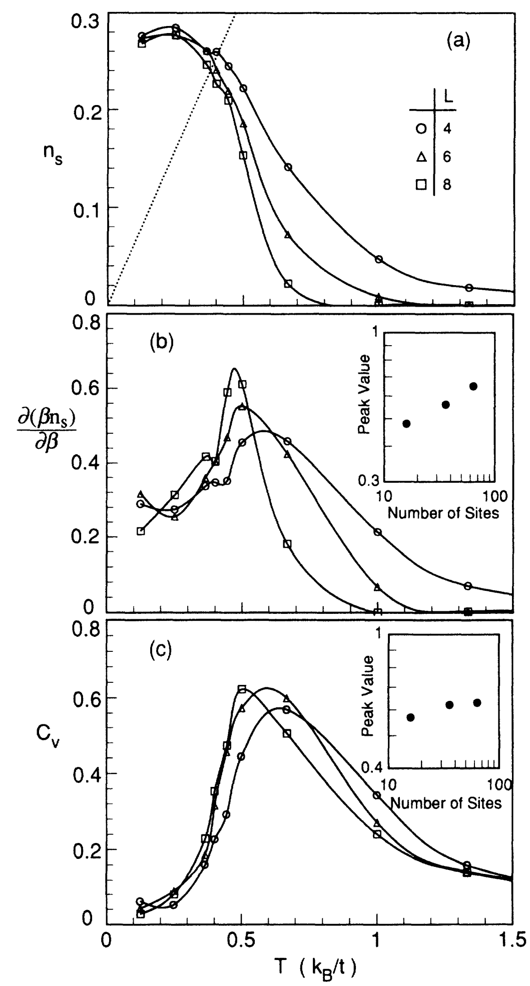


FIG. 1. (a) Two-dimensional superfluid density $n_s$, (b) temperature derivative of $n_s$, and (c) specific heat $C_v$, as a function of temperature $T$, for a clean half-filled system. The symbols denote the cases for different lattice sizes $L = 4$ (circles), 6 (triangles), and 8 (squares). The solid curves represent spline fits to the calculated data. The dotted line in (a) corresponds to the universal jump condition of the Kosterlitz-Thouless transition.

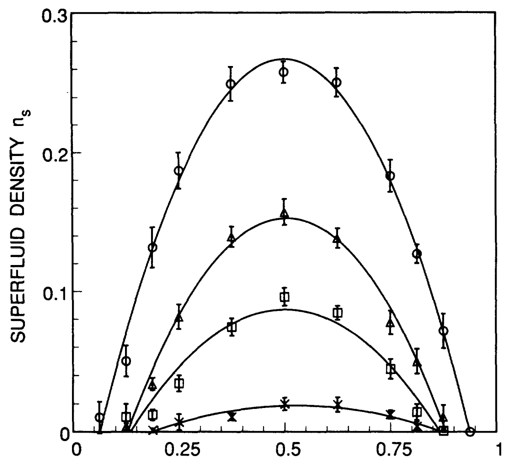


FIG. 2. Low-temperature superfluid density as a function of boson particle density, for different degrees of disorder. This simulation was performed at low temperature $T = 0.25\,t/k_B$ on an $8\times8$ lattice. Each value denotes the thermal and sample averages over five different disordered states. The degrees of disorder are denoted by circles for the clean system ($\Delta = 0$), triangles ($\Delta = 1.0$), squares ($\Delta = 1.25$), and crosses ($\Delta = 1.75$). The solid lines represent parabolic fits to the calculated data.

reduction of maximum $n_s$ at the half filling. Since the transition temperature $T_{\mathrm{KT}}$ is generally proportional to $n_s(T = 0)$ in the 2D system, the above parabolic property implies that the relation between $T_c$ and particle density takes a universal form, which is accompanied with a common offset density in the disordered case.

The disorder always localizes bosons to suppress the superfluidity. Nevertheless the disorder-induced localization appears to differ qualitatively between dense and dilute Bose systems in two dimensions. Figure 3 shows the dependence of $n_s$ on disorder ($\Delta$) at a fixed low temperature. The superfluidity of the moderately dense (half-filled) system is insensitive to weak disorder. At stronger disorder $\Delta \gtrsim 2.5$, the superfluidity disappears, but the size dependence is very weak even when the disorder is rather strong. This result is consistent with earlier studies[13,18] which support the existense of the Bose glass phase for dense systems. In contrast, the dilute system at 1/8 filling ($n_b = 1/8$) is rather sensitive even to weak disorder. Here $n_s$ is rapidly suppressed as the lattice size is increased. This size dependence implies that the correlation length of superfluidity is smaller than the lattice size $L = 8$. The insets of the figure show the spatial distribution of boson density in each case. For the dilute region in the vicinity of $n_b = n_0$, most bosons appear to form a superfluid cluster, as depicted in the upper inset. The size of the cluster is comparable to the localization length $\xi_l$ of the Anderson transition. For instance, using $\xi_l = a/\ln(\Delta/t)$ in the limit of strong disorder, $\xi_l \approx 5a$ for $\Delta = 1.25$. This observation indicates that the 2D weak localization is dominant at densities below $n_0$. On the other hand, for a half-filled system with strong disorder, such clusters assemble into a percolative network, as shown in the lower inset. This behavior is supposed to be associated with critical fluctuations in the vicinity of the Bose glass transition point. Here, when the glass correlation length, larger than the Anderson's localization length, exceeds the lattice size, the superfluidity disappears. By varying the particle density under the hard-core condition, we have thus obtained a possible tuning from Anderson glass to Bose glass in two dimensions. It is interesting that the similar tuning was previously observed in 1D disordered soft-core boson system ($n_b$=0.625) by varying the strength of on-site repulsion from zero (free) to strong (hard-core) couplings.[19]

We made a semiquantitative comparison of these numerical results with several results related to high-$T_c$ superconductors. Hereafter we assume bosons to have a linear size equal to the coherence length on the $CuO_2$ plane, $a = \xi_{ab} \simeq 10$ Å. Recently Matsuda *et al.*[20] carried out transport measurements which provided unequivocal evidence of the KT transition in a one-unit-cell(12 Å)-thick

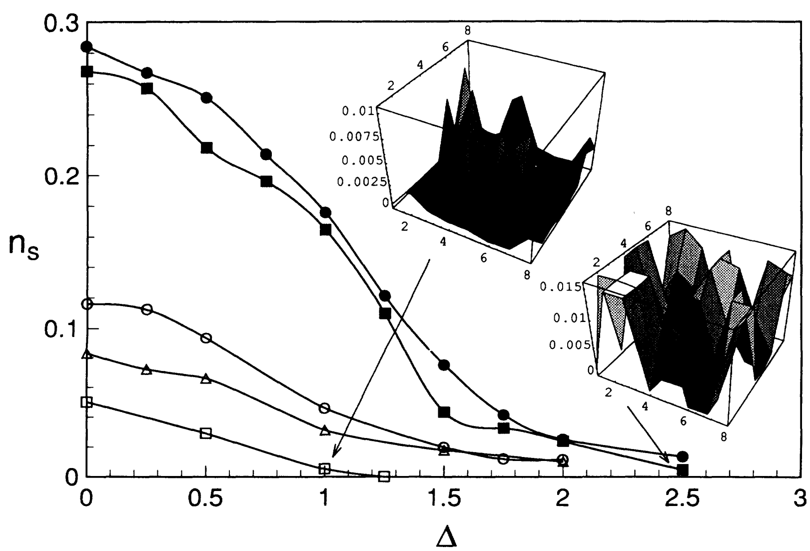


FIG. 3. Localization in dense ($n_b = 1/2$) and dilute ($n_b = 1/8$) Bose systems. The curves show the low-temperature superfluid density as a function of disorder strength, at a fixed temperature $T = 0.25\,t/k_B$. The symbols correspond to lattice sizes $L = 4$ (black circles), 8 (black squares) for the dense system, and $L = 4$ (circles), 6 (triangles), 8 (squares) for the dilute system. The two insets represent the density distribution of bosons on the $8 \times 8$ lattice. The upper and lower insets correspond to the cases of ($n_b = 1/8, \Delta = 1.0$) and ($n_b = 1/2, \Delta = 2.5$), respectively.

$YBa_2Cu_3O_{7-x}$ (YBCO) film with a maximum value of $T_{KT} = 30$ K. The three-dimensional interlayer coupling, thus, is not a necessary condition for finite-$T_c$ superconductivity, although the interlayer coupling plays an additional role in elevating the $T_c$.[21] By comparing the experimental and numerically determined values of $T_{KT}$ in the clean half-filled system $(2m_b^* \xi_{ab}^2 k_B T_{KT}/\hbar^2 \simeq 0.4)$, we estimate the boson mass as $m_b^* = 2m_{\rm carrier}^* \simeq 5.9m_e$, which is comparable to the value of $m_{\rm carrier}^* \simeq 2.5m_e$ given by Schlesinger *et al.*[22] from infrared measurements of YBCO.

In high-$T_c$ superconductors, chemical doping not only results in carrier-density modulation, but also introduces some degree of microscopic disorder in the superconductive $CuO_2$ plane, although the latter effect has not been well elucidated experimentally. One remarkable feature commonly observed in experimental data is that the relationship between the transition temperature $T_c$ and the hole density $\delta$ (per unit cell) follows a common bell-type curve: $T_c(\delta)$ rises above $\delta_{\rm offset} \simeq 0.05$, reaches a maximum at $\delta_{T_c({\rm max})} \simeq 0.18$, and falls down to zero at $\delta_{\rm end} \simeq 0.3$. In addition, the $T_c$-$\delta$ curve is symmetric about $\delta = \delta_{T_c({\rm max})}$, possibly implying some hidden symmetry. These experimental features strongly correlate with the results presented in Fig. 2. Furthermore we theoretically obtained the universal parabolic curve, similar to the ansatz proposed in Ref. 2. By simply assuming that the boson particle density scales with hole density as $n_b = (\delta/2)(\xi_{ab}/l_{ab})^2$ with a unit cell size $l_{ab} \simeq 4$ Å, we get $n_b \simeq 0.16$, 0.56, and 0.94 for $\delta_{\rm offset}$, $\delta_{T_c({\rm max})}$, and $\delta_{\rm end}$, respectively. This is also consistent with the computational results. Thus, the existence of parabolic symmetry and the consistency of characteristic values of $m_b^*$ and $\delta$ strongly suggest that superconductivity within individual $CuO_2$ layers is caused by 2D superfluidity of local bosons moving in somewhat disordered media.

To summarize, our quantum Monte Carlo simulations have provided further support that the 2D hard-core Bose gas undergoes a KT transition to become superfluid, and that the low-temperature superfluid density shows a paraboliclike dependence on particle density. In disordered systems, we have shown that the bosons localize differently in the dense and dilute cases. The computational results correlate with the $T_c$ vs $\delta$ relationship for high-$T_c$ superconductors and may partially illustrate the nature of the superconducting transition.

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[1] Y. J. Uemura *et al.*, Phys. Rev. Lett. **62**, 2317 (1989).
[2] T. Schneider and H. Keller, Phys. Rev. Lett. **69**, 3374 (1992); Physica C **207**, 366 (1993).
[3] H. Zhang and H. Sato, Phys. Rev. Lett. **70**, 1697 (1993).
[4] M. P. A. Fisher, P. B. Weichman, G. Grinstein, and D. S. Fisher, Phys. Rev. B **40**, 546 (1989).
[5] T. Matsubara and H. Matsuda, Prog. Theor. Phys. **16**, 569 (1956).
[6] E. Loh, Jr., D. J. Scalapino, and P. M. Grant, Phys. Rev. B **31**, 4712 (1985).
[7] M. Marcu, in *Quantum Monte Carlo Methods in Equilibrium and Nonequilibrium Systems*, edited by M. Suzuki (Springer, Berlin, 1987), p. 64.
[8] T. Onogi, S. Miyashita, and M. Suzuki, in *Quantum Monte Carlo Methods in Equilibrium and Nonequilibrium Systems* (Ref. 7), p. 75.
[9] M. S. Makivić, Phys. Rev. B **46**, 3167 (1992); M. S. Makivić and H.-Q. Ding, *ibid.* **43**, 3562 (1991); H.-Q. Ding and M. S. Makvić, *ibid.* **42**, 6827 (1990).
[10] J. M. Kosterlitz and D. J. Thouless, J. Phys. C **6**, 1181 (1973); J. M. Kosterlitz, *ibid.* **7**, 1046 (1974).
[11] B. J. Alder and D. S. Peters, Europhys. Lett. **10**, 1 (1989).
[12] W. Krauth and N. Trivedi, Europhys. Lett. **14**, 627 (1991).
[13] K. J. Runge, Phys. Rev. B **45**, 13136 (1992).
[14] To breakup the partition function according to the Suzuki-Trotter transformation, we used the checkerboard type of real-space decomposition of $H_{\rm spin}$ according to Refs. 6 and 7; $Z = {\rm Tr}\, e^{-\beta H} \approx {\rm Tr}\, (e^{-\Delta\tau H_1} e^{-\Delta\tau H_2})^{\beta/\Delta\tau}$ with $n = \beta/\Delta\tau$ time slices, where the Hamiltonian is decomposed into two kinds of cell (four-spin) Hamiltonians $H = H_1 + H_2$ such that they do not overlap. This formula is accurate up to $O(\Delta\tau^2)$. We fixed $\Delta\tau = 1/4$, and performed $(1\text{-}4)\times 10^4$ lattice sweeps after $10^3$ sweeps of thermalization, typically for a single run. The systematic error in the Trotter approximation $\Delta\tau$ is smaller than the statistical error of a few percent.
[15] E. L. Pollock and D. M Ceperley, Phys. Rev. B **36**, 8343 (1987).
[16] J. E. Van Himbergen and S. Chakravarty, Phys. Rev. B **23**, 359 (1981).
[17] E. Lieb, Ann. Phys. **16**, 407 (1961).
[18] W. Krauth, N. Trivedi, and D. M. Ceperley, Phys. Rev. Lett. **67**, 2307 (1991).
[19] R. T. Scalettar, G. G. Batrouni, and G. T. Zimanyi, Phys. Rev. Lett. **66**, 3144 (1991).
[20] Y. Matsuda *et al.*, Phys. Rev. Lett. **69**, 3228 (1992).
[21] Y. Matsuda *et al.*, Phys. Rev. B **48**, 10498 (1993).
[22] Z. Schlesinger *et al.*, Phys. Rev. Lett. **65**, 3228 (1990).

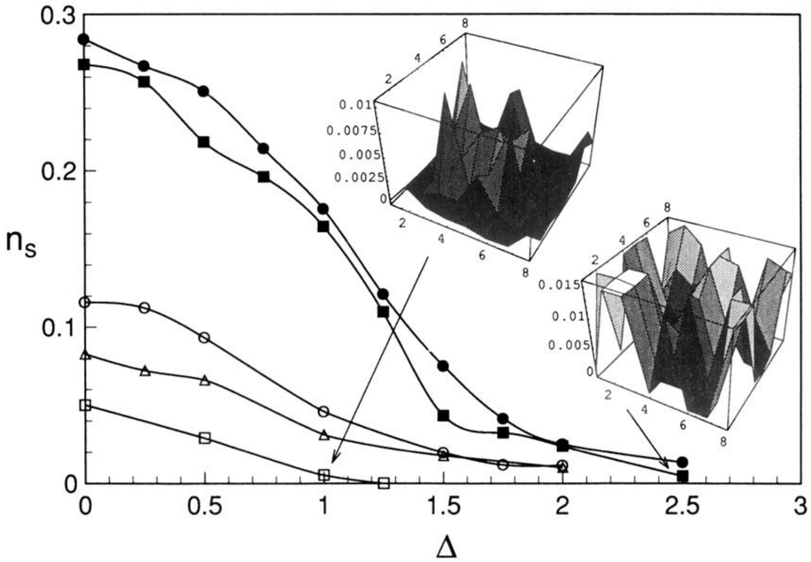


FIG. 3. Localization in dense ($n_b = 1/2$) and dilute ($n_b = 1/8$) Bose systems. The curves show the low-temperature superfluid density as a function of disorder strength, at a fixed temperature $T = 0.25\,t/k_B$. The symbols correspond to lattice sizes $L = 4$ (black circles), 8 (black squares) for the dense system, and $L = 4$ (circles), 6 (triangles), 8 (squares) for the dilute system. The two insets represent the density distribution of bosons on the $8 \times 8$ lattice. The upper and lower insets correspond to the cases of ($n_b = 1/8$, $\Delta = 1.0$) and ($n_b = 1/2$, $\Delta = 2.5$), respectively.