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Trapping Collapse: Infinite Number of Repulsive Bosons Trapped by a Generic Short-ranged Potential

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Weak potential wells (or traps) in one and two dimensions, and the potential wells slightly deeper than the critical ones in three dimensions, feature shallow bound states with localization length much larger than the well radii. We address a simple fundamental question of how many repulsively interacting bosons can be localized by such traps. We find that under rather generic conditions, for both weakly and strongly repulsive particles, in two and three dimensions—but not in one-dimension!—the potential well will trap infinitely many bosons. For example, even hard-core repulsive interactions do not prevent this "trapping collapse" phenomenon from taking place. A quantum system acquires the phenomenon along with the universal (asymptotically exact) classical-field behavior at large distances, allowing generic description by the Gross-Pitaevskii equation. We also discuss the possibility of having a transition between the infinite and finite number of trapped particles when strong repulsive inter-particle correlations are increased.

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Everyone is familiar with the standard quantum mechanical problem of finding bound states in a potential well ("trap") of radius R_0—for simplicity, we assume that the potential is spherically symmetric—in one, two, and three dimensions (1D, 2D, and 3D). While in 3D the trap strength V has to exceed some finite critical value V_c to have one bound state, even an arbitrarily weak trap features a shallow bound state in 1D and 2D; i.e., formally, $V_c = 0$ in low dimensions. For $V - V_c \ll 1/mR_0^2$, with m the particle mass (we will refer to this case as a weak trap), the only bound state ψ_1 is extremely "shallow": the binding energy satisfies the condition $E_1 \ll V - V_c$, and the localization length $l = 1/\sqrt{2mE_1}$ (in the units $\hbar = 1$) is much larger than the well radius R_0.

At the single-particle level, the shallow bound state problem is exhaustively treated in textbooks (see, e.g., [1]). However, to the best of our knowledge, the question of how many (strongly) repulsive particles can be localized by a weak trap—and whether the number can be infinite—has not been properly answered [2]. One may immediately deal with two simple cases, depending on the particle statistics and dimension of space. (i) A weak trap cannot bind more than one fermion because even in the absence of interactions, the second fermion has to go to the delocalized state with zero energy by the Pauli principle. Thus the best total energy of a pair is $E_2 = -E_1$, and adding repulsive interactions may only increase it further (as a finite-size effect for a delocalized state). (ii) A dilute repulsive Bose gas in 1D can be mapped onto non-interacting fermions (the so-called Tonks-Girardeau limit) when $U > 1/2ml^2 = E_1$, implying that even for relatively weak ($U \ll V$) interactions, the trap can bind only one particle, regardless of statistics. [In this work, we focus on short-range repulsive interactions characterized by a typical interaction range $R_i \sim R_0$ and potential strength U; its zero-momentum Fourier component will be denoted as $U(0)$ and the s-wave scattering length, where appropriate, as a_s.]

In all other cases, answering the question requires more elaborate considerations, and, for strong interactions, numerical simulations. The main result of this work is the effect of trapping collapse when in both 2D and 3D cases, weak traps bind infinitely many bosons. In the regime of weak interactions, the effect is readily revealed by solving the Gross-Pitaevskii (GP) equation. Remarkably, the phenomenon holds true even when interactions get strong (e.g., for hard-core bosons), as our lattice path-integral Monte Carlo (PIMC) simulations confirm. We explain analytically and illustrate numerically that despite strong correlations at short distances the effect is still associated with the classical-field asymptotic behavior and is thus controllably captured by the GP equation.

The classical-field approach is justified when properties of the ground state do not change significantly when adding/removing one particle. If we want this condition to be satisfied in the trap region then we need to consider what happens when we add the second particle to the textbook single-particle state ψ_1. In 3D, an estimate of the potential energy of repulsion immediately follows from properties of bound s-wave states (their asymptotic decay goes as $\psi_1 = 1/r\sqrt{4\pi l}$):

$$U_i \approx \frac{4\pi a_s}{m} \int d^3r |\psi_1(\mathbf{r})|^4 \sim \frac{a_s}{ml^2} \int_{R_0} \frac{dr}{r^2} \sim E_1 \frac{a_s}{R_0}. \quad (1)$$

This leads to the following condition for applicability of the classical-field description in the vicinity of the trap

$$a_s \ll R_0 \qquad (3D). \tag{2}$$

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

Once $N \gg 1$ particles are placed on the orbital, the N-body state will start evolving towards a more delocalized density profile because the ionization potential defined in terms of a difference between the total N-particle energies as $I_N = E_{N-1} - E_N$ will approach zero. Justification of the classical-field description at large scales in this case (regardless of what happens in the vicinity of the trap) is now based on the standard two-fold criterion—degeneracy + weak interaction (see, e.g., [5])—formulated as the requirement that the number of particles in the correlation volume $\sim \lambda^d$ be much larger than unity. [Here $\lambda \equiv \lambda(r)$ is the position-dependent de-Broglie wavelength and d is the dimensionality.] For the power-law decaying solution derived below λ is on the order of the distance from the trap center and the degeneracy condition requires that $\int_{r=\lambda}^{r=2\lambda} d^3r|\psi(r)|^2 \gg 1$. The regime of weak interaction is trivially satisfied due to vanishing $\psi(r \to \infty)$.

To see whether the number of localized particles can be infinite, we resort to the stationary GP equation, presuming that the classical matter-field description at large scales is valid. The potential of interest has a ground state $E_0 < 0$ for one quantum particle, meaning that a trapped solution of the stationary GP equation exists for any chemical potential $\mu \in (E_0, 0]$. We are interested in the case $\mu = 0$, in which the amount of trapped matter is either maximal, or divergent. Corresponding GP equation reads: $\Delta\psi(r) = 8\pi a_s\, \psi^3$, or

$$\psi''(r) + 2\psi'(r)/r = 8\pi a_s\, \psi^3\,. \tag{3}$$

The (decaying at large distance) asymptotic solution, $\psi(r \to \infty) = 1/\sqrt{16\pi a_s \ln(r/R_0)}\, r$, features the divergent—at the upper limit—integral for the total particle number, $N = \int d^3r|\psi(r)|^2 \propto \int dr/\ln(r/R_0)$. One can immediately verify that justification criteria are satisfied by this solution in the limit of $\lambda \to \infty$. This establishes the effect of trapping collapse for any 3D quantum system featuring the weakly interacting regime at a certain large scale of distance. As for the total interaction energy, the integral $\int d^3r|\psi(r)|^4$ is still dominated by the trap potential region.

Similar considerations apply to the 2D case with one notable exception: the effective repulsive interaction is now scale-dependent with logarithmic renormalizion towards smaller value at low energies:

$$U_{\rm eff}(k) \approx \frac{U(0)}{1 + g\ln(1/kR_i)}\,, \qquad g = \frac{mU(0)}{2\pi}\,, \tag{4}$$

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

$$U_{\rm i} \approx U_{\rm eff}(1/l) \int d^2r|\psi_1(\mathbf{r})|^4 \sim E_1 mU_{\rm eff}(1/l)\,. \tag{5}$$

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

$$\psi''(r) + \psi'/r = 2mU_{\rm eff}(r)\, \psi^3\,, \tag{6}$$

has the asymptotic form $\psi(r \to \infty) = \sqrt{\ln(r/R_0)/4\pi}/r$. Here we explicitly consider the universal asymptotic expression for $mU_{\rm eff}$. If the value of the constant g in Eq. (4) is small, and the logarithmic flow of the coupling constant can be neglected, then in a broad range of intermediate length scales the solution is simply $\psi(r) = 1/\sqrt{4\pi g}\, r$. Again, the integral for the total particle number diverges at the upper limit, $N \propto \int dr \ln(r/R_0)/r$, indicating that weak traps in 2D can localize infinitely many bosons, including strongly repulsive ones. [Logarithmic dependence of N on the upper cutoff ensures that finite-density corrections to the $U_{\rm eff}(r)$ dependence on length scale remain sub-leading.] As in 3D, the condition of degeneracy is guaranteed to be met in the $r \to \infty$ limit. Observe, however, the crucial role of the vanishing coupling strength.—The asymptotically exact classical-field description in 2D is more subtle than in 3D!

To illustrate these results—especially under the conditions of strong correlations at short distances, we resort to lattice PIMC simulations [5] of square/cubic lattice systems with tight-binding dispersion relation $\epsilon(\mathbf{k}) = 2t\sum_{\alpha=1}^{d}[1 - \cos(k_\alpha a)]$, where t is the nearest-neighbor hopping matrix element and a is the lattice constant (in what follows, the energy and distance are measured in units of t and a, respectively). The trap is introduced as an attractive potential $-V\delta_{\mathbf{r},0}$ placed at the origin. The repulsive pairwise interactions between particles are of the on-site Hubbard form, $U(\mathbf{r}_i - \mathbf{r}_j) = U\delta_{\mathbf{r}_i-\mathbf{r}_j,0}$. In 2D, our study of localized many-particle states was performed for $V = 2$ to ensure that the binding energy is about a factor of one hundred smaller than the bandwidth, $E_1 = 0.0576$. The critical value of V for forming a bound state in a cubic lattice is $V_c = 3.956776$; for the trapping potential strength $V = 4.3$ used in this work the binding energy is only $E_1 = 0.06058$.

In Figs. 1 – 4, we show data for localized density profiles of multi-particle states in weak traps. The data are

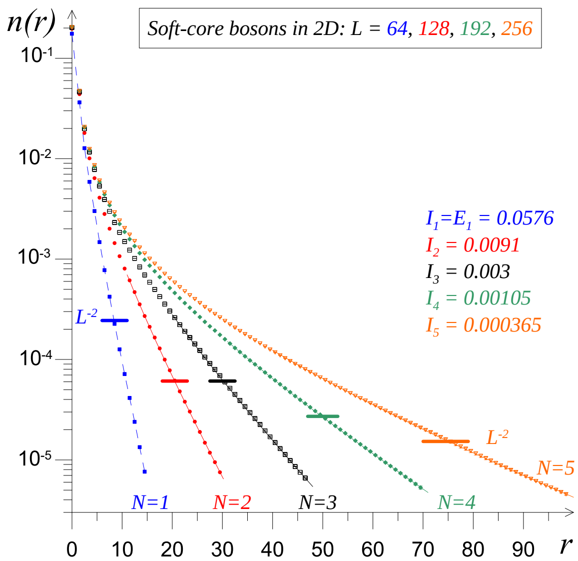

FIG. 1: (color online). Radial density profiles in 2D for $V = -2$ and $U = 4$ at $\beta = 16000$. System sizes were increased for larger N to ensure that $n(r)$ for weakly bound states drops well below the L^{-2} level (shown by the bold bar) characteristic of a delocalized single-particle state. Error bars are smaller than symbol sizes unless shown explicitly. Solid fitting lines are explained in the text.

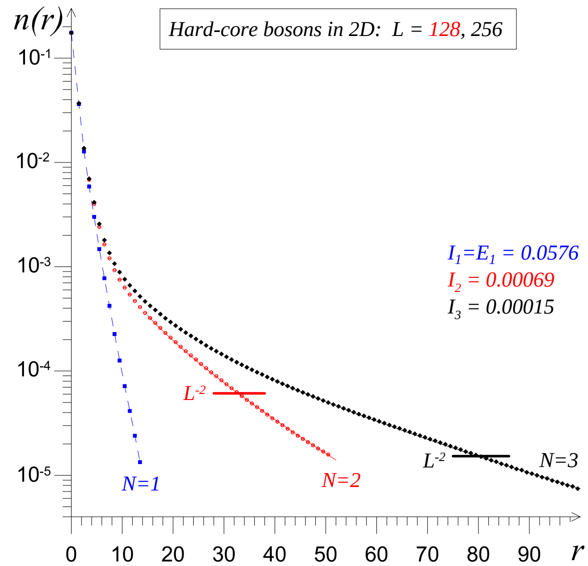

FIG. 2: (color online). Radial density profiles for hard-core bosons in 2D for $V = -2$ at $\beta = 16000$ (see Fig. 1 caption for additional details that are identical for both figures).

averaged over circular/spherical bins of unit length in the radial direction. With the Monte Carlo algorithm optimized for simulations of dilute systems, when hundreds of kinks are changed in a single elementary update, we were able to address ground state properties of very large systems (in all fixed-N simulations the inverse temperature $\beta = 1/T$ was large enough to guarantee that contributions from excited states were negligible). As the localization length rapidly increases with the number of particles, we ultimately hit the computational complexity threshold at some finite N. In 2D, for inter-particle repulsion strength $U = 4$, we were able to quantify properties of localized states of up to five bosons, see Fig. 1. Clearly, having the inter-particle repulsion a factor of two stronger than the trap potential does not stop the system from forming a localized many-body ground state.

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

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

We find similar results for 3D systems, see Fig. 3. For $U = 1$ (relatively weak coupling) the two-particle bound state resembles that of two bosons being placed on the same orbital, but even then the ionization potential is about a factor of six smaller than E_1. For $U = 3$ we are already dealing with the ground state where positions of two particles are strongly correlated. For hard-core bosons, we certainly violate the condition (2), and the two-body state develops a signature bi-model shape when at short distance the two-body density profile is closely following a single particle one, see Fig. 3. This appears to be the generic mechanism for particles to minimize ef-

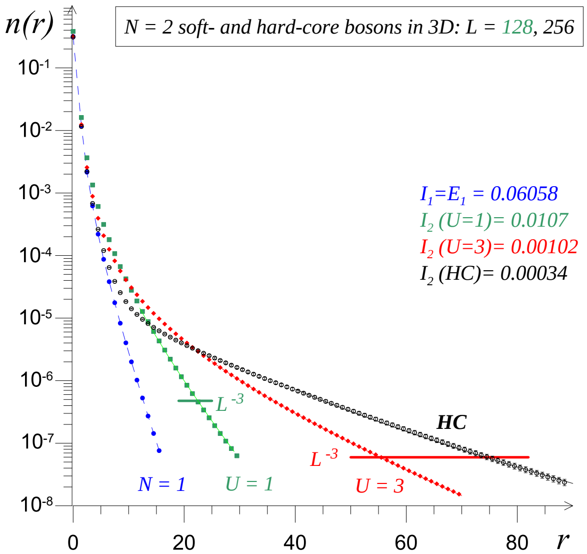

FIG. 3: (color online). Radial density profiles for two soft- and hard-core bosons in 3D for $V = -4.3$ at $\beta = 10000$. The L^{-3} level characteristic of the delocalized single-particle state is shown by bold bars. Large scale decays are fitted to the $e^{-2r/l_2}/r^2$ law.

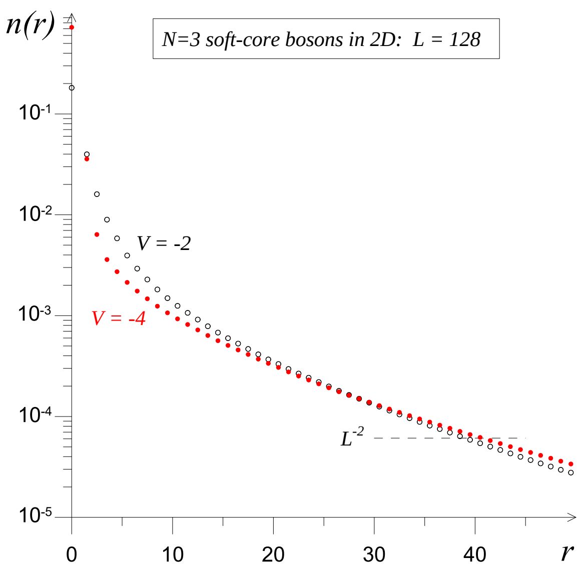

FIG. 4: (color online). Radial density profiles for three bosons in 2D for $U = 10$ in traps with $V = 2$ and $V = 4$ at $\beta = 4000$, showing that the state is more localized in a weaker trap.

fects of strong repulsive interactions while gaining enough potential energy from the trap to remain in the localized state. The energy balance, however is extremely delicate: the ionization potential $I_2(HC)$ is nearly two hundred times smaller then E_1!

The most intriguing question that remains unanswered by the data, is the transition, if any, between the ground state with infinitely many localized particles and a state with a few, or just one, localized particles as the range and strength of the repulsive interaction is increased, or, counter-intuitively, when the trap potential is increased. Indeed, according to expression (4), effects of repulsive interactions are more pronounced for smaller localization length l, or deeper traps. Strong-correlation effects then result in a state where one particle stays close to the trap center and effectively "screens" it out. This effect is verified and quantified in Figs. 4 and 5 using two different setups. In Fig. 4, we directly observe that the state of three bosons with strong on-site repulsion $U = 10$ is more delocalized in a deeper trap with $V = 4$ than in a trap with the shallow single-particle state at $V = 2$.

Higher energies for multi-particle states in a deeper trap imply that the average particle number at a given temperature and zero chemical potential must have a minimum at some value of V (when V is larger than U, one tightly localized particle can no longer fully screen the trap). Minima on the $\langle N \rangle$ curves as a function of V for 2D soft-core boson with $U = 10$ are clearly seen in Fig. 5. As far as evidence goes, increasing trap potential for strongly repulsive bosons with $U = 10$ does not lead to the trapping collapse transition: we do not observe saturation of the $\langle N \rangle$ curves to some finite thermodynamic limit answer when the system size is increased (temperature is decreased accordingly to keep the product $TL^2 = 8$ fixed), see Fig. 5.

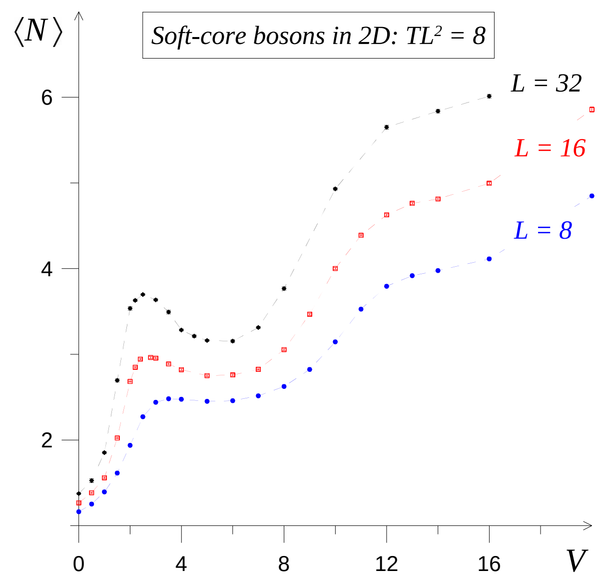

FIG. 5: (color online). Average number of soft-core bosons with $U = 10$ at zero chemical potential as a function of trap strength for different system sizes and temperatures in 2D.

In conclusion, we have found that two- and three-dimensional finite-range potential wells, including those featuring only one weakly bound single-particle state, will localize infinitely many bosons even when repulsive inter-particle interactions are much stronger than the trapping potential. We termed this effect the trapping collapse, tracing its origin in the classical-field long-wave behavior captured by the Gross-Pitaevskii equation. Future work should clarify whether and under what conditions the trapping collapse phenomenon may be replaced with localization of a finite (one ?) number of particles and what are properties of systems at the transition point. Our results may find important applications in studies of Bose-Einstein condensates in atomic and solid state systems, especially in disordered systems.

We are grateful to E. Kolomeisky for bringing Refs. [3, 4] to our attention. We thank Panayotis Kevrekidis for the discussion of our results.

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