

Quantum Many-Body Culling: Production of a Definite Number of Ground-State Atoms in a Bose-Einstein Condensate

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We propose a method to produce a definite number of ground-state atoms by adiabatic reduction of the depth of a potential well that confines a degenerate Bose gas with repulsive interactions. Using a variety of methods, we map out the maximum number of particles that can be supported by the well as a function of the well depth and interaction strength, covering the limiting case of a Tonks gas as well as the mean-field regime. We also estimate the time scales for adiabaticity and discuss the recent observation of atomic number squeezing [Chuu *et al.*, Phys. Rev. Lett. **95**, 260403 (2005)].

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The controlled generation of many-body atomic number states has been a long-standing goal in physics, and success would provide an enabling tool for the study of entanglement [1–4] and few-body tunneling [5] with possible applications in quantum computing. One avenue towards this goal is the Mott insulator state where single-atom or multi-atom number states are predicted [6,7]. Current experiments along this line are based on optical lattices [8] where direct access to individual sites has not been accomplished and appears very difficult. A completely different approach was taken in a recent experiment where number squeezing was created and observed by direct atom counting [9]. Motivated by this work, we have studied theoretically the question of number-state generation, and the results are presented in this Letter. We find that number-state generation is indeed possible, and we identify appropriate parameter regimes and conditions for its realization.

The basic idea is to confine a degenerate Bose gas in an optical box with a finite barrier height that can be controlled. The repulsive interaction between the atoms implies that a finite box can only contain a maximum number of atoms. As the barrier height is slowly reduced, atoms must leave, and the final number is completely determined by the stopping point of the barrier. Since the confinement and the barrier in Ref. [9] were realized by means of optical dipole traps, we call this process “laser culling of atoms” although the same principle could also be implemented in other types of traps. The main theoretical questions that must be addressed are how the maximum number of atoms depends on the potential and interaction strength and how slowly must the potential be changed in order to avoid excitations within the box. Below, we outline the idea of atomic culling in two limiting cases: impenetrable bosons in one extreme and a modified mean-field picture in the other. The diffusion Monte Carlo and direct diagonalization of the Hamiltonian bridge these two regimes. Finally, we discuss the criteria for adiabaticity of the process.

Maximum number of bound atoms—Consider a one-dimensional model of N bosons in a square well of depth V_0 and width L , interacting with each other with a delta function potential of strength g . This is the simplest model of the potential well used in Ref. [9], when the lateral directions are tightly bound and tunneling through the barriers is negligible. The experimental system had a lateral confinement frequency of about $\nu_{\perp} = 200$ Hz, which is not high enough to make the system truly one-dimensional. However, much stronger confinement may be employed in the future ($\nu_{\perp} = 40$ kHz has been achieved recently). We use dimensionless units with Planck’s constant \hbar , atomic mass m , and the well width L set to unity. There are only two dimensionless parameters in our model, the well depth in units of $(\hbar/L)^2/m$ and the interaction strength in units of \hbar^2/mL . The dimensionless interaction strength may be conveniently written as $g = 4\pi\nu_{\perp}ma_sL/\hbar$ [10], where a_s is the scattering length. For ^{87}Rb confined in a well of $L = 10 \mu\text{m}$ with $\nu_{\perp} = 1$ kHz of lateral confinement, one has $g \approx 1$. Such a system would be in the weak coupling regime (defined by $g \ll N$) for all but a very small number of atoms.

An obvious approach in the weak coupling regime is the mean-field approximation assuming that all N particles occupy the same single-particle state, with its wave function determined variationally by the Gross-Pitaevskii (GP) equation [11,12]. However, this approximation is only good for the case when all particles are deeply bound in the well. Near the “ionization” threshold, one particle should become weakly bound with long tails of its wave function extending beyond the well, while all others remain tightly bound. This situation is more appropriately described by a Hartree-Fock-type wave function with $N - 1$ particles in a state ϕ_1 and one particle in another state ϕ_2 [13,14]. In order to minimize the total energy, ϕ_1 should be symmetric and nodeless. For bosons, ϕ_2 does not need to be orthogonal to ϕ_1 , and should also be symmetric and

nodeless, because the N -body ground-state wave function should be so with respect to any particle coordinates.

In Fig. 1, we show the result of a variational minimization of the total energy for the case of $N = 3$, and $g = 1$, using trial orbitals of the form

$$\phi_i(x) = \sqrt{\kappa_i} \exp(-\kappa_i|x|) \quad (i = 1, 2). \quad (1)$$

When the well is deep, κ_i are all comparable, indicating the tendency for all particles to occupy a single state. As the well becomes shallow, κ_2 tends to zero while κ_1 remains finite, which corresponds to delocalization of only one particle. For comparison, we have also calculated the total energy when only a single orbital is used (by setting $\kappa_1 = \kappa_2$), finding a higher ground-state energy.

Without the orthogonality condition, the equations for determining the optimal form of the orbitals are complicated. Fortunately, at ionization threshold, the two orbitals are orthogonal because ϕ_2 becomes extended. Minimization of the Hartree-Fock energy leads to the coupled nonlinear equations

$$\begin{aligned} [h(x) + g(N-2)|\phi_1|^2 + 2g|\phi_2|^2]\phi_1 &= \mu_1\phi_1, \\ [h(x) + 2(N-1)g|\phi_1|^2]\phi_2 &= \mu_2\phi_2, \end{aligned} \quad (2)$$

where $h(x)$ is a single-particle Hamiltonian. The first equation reduces to the GP equation for $N-1$ particles because the amplitude of ϕ_2 is negligible at the ionization threshold. The second equation describes a particle in the effective potential of the square well plus the mean-field potential of the $N-1$ particles. The ionization condition ($\mu_2 = 0$) is reached when the integral of the effective potential vanishes, i.e.,

$$V_0 = 2g(N-1)/L. \quad (3)$$

For a potential well which is not a square but is symmetrical, we can still apply the above reasoning, and the result is that $-V_0L$ must be replaced by the integral of the potential. We also note that the GP equation for all N

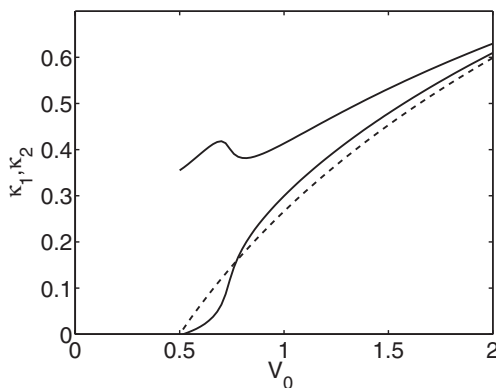


FIG. 1. Calculation of parameters κ_1 and κ_2 from a variational principle for the case of $N = 3$ and $g = 1$. Dashed line shows the result based on a single trial orbital.

particles in a single orbital would yield an erroneous ionization threshold which is only half of the above value.

In the opposite limit of strong interactions, $g \gg N$, we have the case of N impenetrable bosons. The problem is mapped to N noninteracting fermions in a square well [15]. The many-body eigenstates of the problem are given by the absolute value of the Slater determinant of single-particle states. The potential well can support N bound single-particle states when the well is deeper than

$$V_0 = [\pi(N-1)/L]^2/2; \quad (4)$$

only then can N impenetrable bosons be trapped. As the well depth decreases to such a value that the most energetic single-particle state delocalizes, only $N-1$ particles remain trapped in the well, as illustrated in Fig. 2. We note that the Tonks gas limit is physically quite different than the regime of Ref. [9], where $g = 0.2$.

To solve the problem for intermediate values of g , we resort to a direct diagonalization of the many-body Hamiltonian. In order to execute numerical calculations, we contain the well in a large box of size $D \gg L$ with hard walls and find single-particle eigenstates. A discrete second-quantized Hamiltonian is then constructed with elements given by the eigenenergies and by integrals of products of the eigenfunctions. An N -body Hamiltonian matrix can then be formed in the Fock-state basis and is diagonalized by standard numerical routines. The bound-state total energies for $N = 1, 2, 3$, and $g = 1$ are shown in Fig. 3 for different V_0 .

As an alternative method to calculating the ground state of N bosons, we use the diffusion Monte Carlo approach [16]. Previously, this method was successfully used to calculate the ground state of bosons with an arbitrary interaction strength. With this approach, we also take a box of size $D \gg L$. In Fig. 4, we show threshold values of the well depth above which N particles can be supported. Statistical errors are estimated to be comparable to the size

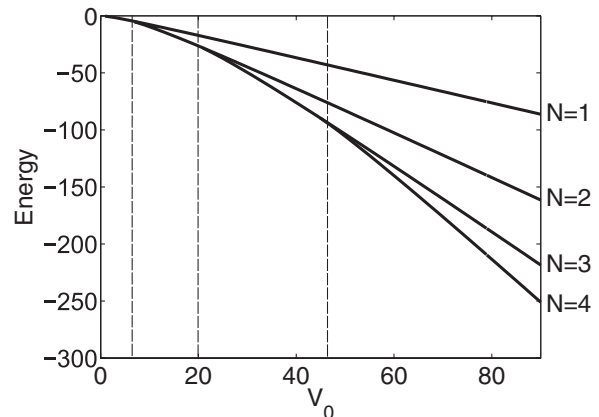


FIG. 2. Ground-state energy of N Tonks bosons in a square well as a function of well depth. Zero of energy is at the top of the well. Whenever two energy levels merge (as denoted by three vertical dashed lines), a particle is ionized.

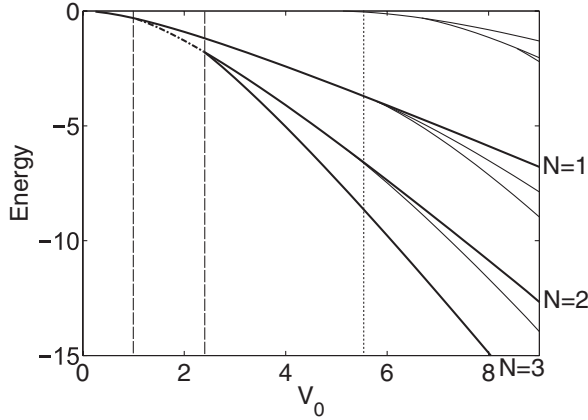


FIG. 3. Bound levels of bosons interacting with $g = 1$. Zero of energy is at the top of the well. Thick lines correspond to ground state of N particles. Thin lines indicate bound excitations. Two vertical dashed lines indicate the region where only $N = 1, 2$ particles are supported in the bound-state. Vertical dotted line shows the smallest V_0 for which an excited bound-state is supported for $N = 3$.

of the symbols (except for the case of $N = 4$ at $g = 4$). Results for $N = 1, 2, 3$ at $g = 1$ agree very well with direct diagonalization. Results in the weak coupling regime $g \ll N$ are predicted correctly by the formula Eq. (3).

Adiabaticity condition—We now discuss how to achieve the atomic number states that we have studied above. We assume that our initial state is one with an unknown number of atoms but at essentially zero temperature. Since our eventual goal is to obtain a few atoms with a known definite number, this initial ensemble can be rather small, containing, say, about 100 atoms. It can be prepared

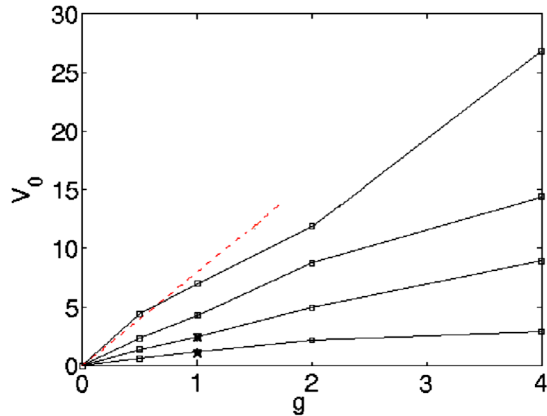


FIG. 4 (color online). Ionization threshold values of the well depth as functions of the interaction strength. Curves from bottom to top are for $N = 1, 2, 3, 4$, respectively. The squares are obtained with a diffusion Monte Carlo method, and the lines are guides for the eye. The two crosses for $g = 1$ are obtained with direct diagonalization. The dashed line is from the weak coupling formula Eq. (3) for the case of $N = 4$.

from a large Bose-Einstein Condensate (BEC), with 10^4 atoms at 10% of the condensation temperature T_c . By maintaining a sufficient density with continuous reduction of the well size, it is certainly possible to reach a temperature of 1% of T_c by further evaporative cooling with about 100 atoms left in the trap [17]. The estimated fraction of thermal atoms will be $(T/T_c)^{3/2} = 0.1\%$, yielding a high probability for all the remaining atoms to be in the ground state. To reach even smaller atom number (towards $N = 1$), the size of the box must be appropriately reduced in order to maintain the high density required for evaporation. This would then ensure that the thermal fraction is negligible and the fidelity of number-state generation is very high. The techniques for making a single tightly-confined optical box were developed by us and described in two earlier papers [18].

At this stage, the atomic number may not be the maximum allowed for the potential well because atoms with energies near the top of the barrier may be “ionized” due to various perturbations. As long as the atomic gas is not excited within the well, we can regard our system to be in a ground state, albeit with an unknown number of atoms. Towards this goal, the perturbations have to be small compared to the excitation energy gap. In the weak coupling limit, the latter can be estimated to be the Bogoliubov excitation of the longest wavelength [19], $\hbar\omega = (\rho g/m)^{1/2} \pi \hbar/L$, where ρ is the one-dimensional density of atoms. Interestingly, the same expression is obtained even if the system is in the three-dimensional regime, where one only need to take g as the three-dimensional coupling constant divided by the cross sectional area of the atomic gas. For the system studied in the recent experiment [9], a time scale of 5 ms is found for the excitation gap. This is in fact within an order of magnitude of the observed time scale for the onset of nonadiabatic effects on atom number statistics. Deviation from the weak coupling results is important only when g/N (corresponding to γ in Ref. [20]) is large compared to unity. For intermediate couplings, the excitation energy levels are calculated and displayed as thin lines in Fig. 3. In the strong coupling limit, there are no bounded excitations for a maximally bound number of atoms.

As the well size or potential barrier is reduced, it is possible to achieve a state with the atomic number equal to the maximum allowed, provided one can avoid unintended ionizations. Two conditions must be satisfied. First, the precision in the control of well size and barrier height must be within the window between the ionization thresholds. In the weak coupling limit, $g \ll N$, this window size is $\Delta V_0 = 2g/L$. In the strong coupling limit, we have $\Delta V_0 = (N - \frac{1}{2})(\pi/L)^2$. For intermediate couplings, these windows are the gap regions between the lines in Fig. 4 and between vertical lines in Fig. 3.

Second, the ionization energy in the middle of a parameter window (where it is maximum) must be large enough to

withstand noise and nonadiabatic effects. The ionization energy is the difference between N - and $(N - 1)$ -particle states when $N + 1$ particles have stopped being supported. In the weak coupling regime and for a well depth in the middle between two ionization threshold values, we may use the standard GP theory to find the total energies for N and $N - 1$ particles. An analytic result can be obtained in the Thomas-Fermi limit, where the ionization energy is found to be gN/L . In the strong coupling regime and for $N \gg 1$, the ionization energy is found to be $(N + \frac{1}{2})(\pi/L)^2$. For intermediate couplings and small number of particles, the ionization energy is given by the gap between the two lowest thick lines in Fig. 3. Clearly, a stronger interaction strength creates a larger ionization energy.

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