Producing Bose-Einstein Condensates Using Optical Lattices

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We relate the entropies of ensembles of atoms in optical lattices to atoms in simple traps. We then determine which ensembles of lattice-bound atoms will adiabatically transform into a Bose condensate. This shows a feasible approach to Bose condensation without evaporative cooling.

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There is considerable interest in combining weakly interacting Bose-Einstein condensates (BECs) [1] with optical lattices [2]. The BEC-lattice combination is a dream model system: Interactions among atoms in the BEC can be simply parametrized, and the optical lattice potential is exactly calculable. Work to date, both experimental and theoretical, has started with a BEC, and then put it in a lattice. For example, BECs in 1D lattices have been used to make a pulsed atom laser [3] and to demonstrate four wave mixing [4] and squeezing [5] of atoms. The superfluid-Mott insulator transition has been predicted [6] and observed [7] with BEC in a 3D lattice. In this Letter, we theoretically address the converse problem. Atoms that have never been Bose condensed start out deeply bound in a 3D optical lattice. The optical lattice is adiabatically removed, so that the atoms are left in either a flatbottom or a harmonic trap. We determine, via *entropy comparison*, those initial conditions for which the final state is a BEC. Apart from the insight this provides for the types of experiments performed to date, it also presents a strategy for achieving BEC without evaporative cooling. This novel approach to BEC could be orders of magnitude faster than existing techniques and allow for condensation of atomic species otherwise unaccessible via evaporative cooling (e.g., cesium).

We consider only initial lattice distributions with either one or zero atoms per site. These are the most likely distributions after laser cooling in a lattice, because photoassociative collisions efficiently remove pairs of atoms at the same site [8]. We assume that atoms have been optically pumped and are thermally distributed among lattice site vibrational levels, the result of, for instance, 3D Raman sideband cooling in an optical lattice [9,10].

To realize these initial lattice distributions, we assume that atoms are initially trapped with no coupling between the sites and an infinitely strong in-site repulsion. Each site is represented by a three-dimensional harmonic oscillator of frequency ω. We also assume a site-dependent energy offset $\epsilon_{\mathbf{i}} - \frac{3}{2}\hbar\omega$ of the bottom of each harmonic oscillator,

$$\hat{H}_l = \sum_{\mathbf{i}} \sum_{\{j\}} \left(\epsilon_{\mathbf{i}} + \hbar\omega \sum_{\alpha=x,y,z} j_\alpha \right) \hat{n}_{\mathbf{i},\{j\}} + \tilde{\Theta}(\hat{n}_{\mathbf{i}}), \quad (1)$$

where the operator $\hat{n}_{\mathbf{i},\{j\}} \equiv \hat{a}^\dagger_{\mathbf{i},\{j\}} \hat{a}_{\mathbf{i},\{j\}}$ corresponds to the number of atoms in the **i**th site in the "in-site" state given by the $\{j\} \equiv \{j_x, j_y, j_z\}$ set of the "Cartesian" quantum numbers, the operator $\hat{n}_{\mathbf{i}} \equiv \sum_{\{j\}} \hat{n}_{\mathbf{i},\{j\}}$ gives the total number of atoms in the **i**th site, the function

$$\tilde{\Theta}(n) \equiv \begin{cases} 0 & \text{for } n = 0, 1 \\ +\infty & \text{for } n \geq 2 \end{cases} \quad (2)$$

provides the infinite in-site repulsion, and $\hat{a}^\dagger_{\mathbf{i},\{j\}}$ ($\hat{a}_{\mathbf{i},\{j\}}$) is an operator creating (annihilating) a bosonic atom in the **i**th site in the "in-site" state $|\{j\}\rangle$.

In what follows, we will use a grand-canonical expression for the entropy: $S = -\mathrm{Tr}[\ln(\hat{\rho})\,\hat{\rho}]$, where $\hat{\rho} = Z^{-1} \exp[-\beta(\hat{H} - \mu\hat{N})]$ is the grand-canonical N-body density matrix of the system normalized to unity, $Z = \mathrm{Tr}\{\exp[-\beta(\hat{H} - \mu)]\}$ is the partition function, the chemical potential μ is chosen to provide the actual total number of particles N: $\mathrm{Tr}[\hat{N}\,\hat{\rho}] = N$, $\hat{N}$ being the total-number-of-particles operator, and $\beta = 1/T$ is the inverse temperature corresponding to the total energy E of the system: $\mathrm{Tr}[\hat{H}\,\hat{\rho}] = E$.

Generic lattice: entropy.—The total entropy of a lattice is the sum of the entropies of individual sites:

$$S_l = \sum_{\mathbf{i}} \tilde{s}_{\mathbf{i}}, \quad (3)$$

that according to the expression for the entropy given above can be shown to be

$$\tilde{s}_{\mathbf{i}} = \ln(\tilde{z}_{\mathbf{i}}) + \beta(e_{\mathrm{h.o.}} - \mu_{\mathbf{i}})\bar{n}_{\mathbf{i}}. \quad (4)$$

Here $\mu_{\mathbf{i}} = \mu - \epsilon_{\mathbf{i}}$ is the effective chemical potential, $\tilde{z}_{\mathbf{i}} = 1 + e^{\beta\mu_{\mathbf{i}}} z_{\mathrm{h.o.}}$ is the site's partition function, and $z_{\mathrm{h.o.}} = (1 - e^{-\beta\hbar\omega})^{-3}$ and $e_{\mathrm{h.o.}} = 3\hbar\omega\,(e^{\beta\hbar\omega} - 1)^{-1}$ are, respectively, the partition function and energy of a single three-dimensional harmonic oscillator.

For a given temperature and chemical potential, the total number of particles in the lattice is $N = \sum_{\mathbf{i}} \bar{n}_{\mathbf{i}}$, where

$$\bar{n}_{\mathbf{i}} = \frac{e^{\beta\mu_{\mathbf{i}}} z_{\mathrm{h.o.}}}{1 + e^{\beta\mu_{\mathbf{i}}} z_{\mathrm{h.o.}}} \quad (5)$$

is the mean occupation of the site.

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Flat lattice: entropy.—Here we will assume that all the lattice sites have the same energy offset and the number of available sites is N_s:

$$\epsilon_{\mathbf{i}} = 0 \quad \forall\ \mathbf{i} \in [-N_s^{1/3}/2;\ +N_s^{1/3}/2]^3. \tag{6}$$

The computation of the entropy is lengthy but straightforward. It turns out that the entropy per particle $s_l \equiv S_l/N$ (where here and below the index l stands for "lattice") is a universal function of the mean lattice site occupation, $\bar{n} = \frac{N}{N_s}$ (the same for each site), and the probability, w_0, that the ground vibrational state of a given site is occupied if the site itself is occupied (also the same for each site). The entropy per particle is

$$s_l(w_0, \bar{n}) = s_l^{T=0}(\bar{n}) + s_{\text{h.o.}}(w_0), \tag{7}$$

where

$$s_l^{T=0}(\bar{n}) = \bar{n}^{-1}\{(1-\bar{n})\ln[1/(1-\bar{n})] + \bar{n}\ln(1/\bar{n})\} \tag{8}$$

is the entropy per particle in the same lattice but at zero temperature [11], and

$$s_{\text{h.o.}}(w_0) = \frac{3}{w_0^{1/3}}\{{}^{01/3}_{w}\ln(1/w_0^{1/3}) + (1-w_0^{1/3})\ln[1/(1-w_0^{1/3})]\} \tag{9}$$

is the entropy of a single one-particle three-dimensional harmonic oscillator whose ground state is occupied with a probability w_0. Thermal equilibrium is assumed.

Lattice with a harmonic envelope: entropy.—Consider now a lattice whose site ground state energies harmonically depend on the site position:

$$\epsilon_{\mathbf{i}} = \frac{m\Omega^2 l^2}{2} i^2, \tag{10}$$

where l is the distance between the sites assumed to form a cubic lattice. The computation of the harmonic-lattice entropy is pretty analogous to the one for the flat lattice. It leads to

$$s_l(w_0, \bar{n}) = s_l^{T=0}(\bar{n}) + s_{\text{h.o.}}(w_0), \tag{11}$$

where $\bar{n} = \mathrm{Tr}[\hat{n}_{\mathbf{i}=0}\,\hat{\rho}]$ now denotes the site occupation in the center of the lattice,

$$s_l^{T=0}(\bar{n}) = \frac{5\mathrm{Li}_{5/2}(-q(\bar{n}))}{2\mathrm{Li}_{3/2}(-q(\bar{n}))} - \ln[q(\bar{n})], \tag{12}$$

$$q(\bar{n}) = \frac{\bar{n}}{1-\bar{n}} \tag{13}$$

is the entropy per particle at zero temperature, and the three-dimensional harmonic oscillator entropy $s_{\text{h.o.}}(w_0)$ is given above. Here $\mathrm{Li}_\eta(x) \equiv \sum_{j=1}^{\infty} x^j/j^\eta$ is the polylogarithmic function. In the course of the above calculation, we implicitly assumed that the site occupation was a slow function of the site index, and thus the summation over the sites was replaced by an integral.

A general power-law trap: entropy at T_c.—At the end of the thought transfer process atoms are confined in a smooth trap. In what follows, we will assume that many trap levels are populated, so that the semiclassical approximation applies. Within the semiclassical approximation, the number of (noncondensed) particles and the total entropy are given by

$$N_t' = \int d^3\mathbf{r}\, d^3\mathbf{p}\, w(\mathbf{r}, \mathbf{p}), \tag{14}$$

$$S_t = \int d^3\mathbf{r}\, d^3\mathbf{p}\, \sigma(\mathbf{r}, \mathbf{p}), \tag{15}$$

respectively, where the expressions

$$w(\mathbf{r}, \mathbf{p}) = (2\pi\hbar)^{-3}\sum_{n=0}^{\infty} np(n|\mathbf{r}, \mathbf{p}) = (2\pi\hbar)^{-3}\frac{1}{e^{\beta(h_t(\mathbf{r},\mathbf{p})-\mu)}-1}, \tag{16}$$

and

$$\sigma(\mathbf{r}, \mathbf{p}) = (2\pi\hbar)^{-3}\sum_{n=0}^{\infty} -\ln[p(n|\mathbf{r}, \mathbf{p})]\, p(n|\mathbf{r}, \mathbf{p}) = (2\pi\hbar)^{-3}\left\{\ln[z(\mathbf{r}, \mathbf{p})] + \frac{\beta[h_t(\mathbf{r}, \mathbf{p}) - \mu]}{e^{\beta[h_t(\mathbf{r},\mathbf{p})-\mu]}-1}\right\} \tag{17}$$

are the particle- and entropy phase-space densities, and

$$p(n|\mathbf{r}, \mathbf{p}) = z(\mathbf{r}, \mathbf{p})^{-1} e^{-\beta[h_t(\mathbf{r},\mathbf{p})-\mu]n}, \tag{18}$$

$$z(\mathbf{r}, \mathbf{p}) = \sum_{n=0}^{\infty} e^{-\beta[h_t(\mathbf{r},\mathbf{p})-\mu]n} \tag{19}$$

are the distribution of the number of particles in a volume $(2\pi\hbar)^3$ phase-space cube centered at a point $(\mathbf{r}, \mathbf{p})$, and the corresponding partition function. Bose-Einstein condensation occurs as soon as the total number of particles exceeds the upper bound for the number of the noncondensed particles $N^\star \equiv N'|_{\mu=0}$ given by its value at zero chemical potential [12]:

$$N \geq N^\star \Longleftrightarrow \text{BEC} \tag{20}$$

(see [12] for an extension of the concept of Bose-Einstein condensation to the case of a general power-law trap). Below, we will reformulate this condition in terms of the entropy per particle $s_t = S_t/N$.

Consider a general power-law trapping potential,

$$U(\mathbf{r}) = \sum_{\alpha=x,y,z} a_\alpha (r_\alpha)^{\lambda_\alpha}. \tag{21}$$

After lengthy but straightforward calculations, one can show that in this case the critical entropy per particle assumes a universal form:

$$s_t^\star = \frac{S_t^\star}{N^\star} = \frac{(\eta+2)\zeta(\eta+2)}{\zeta(\eta+1)}, \tag{22}$$

where $\eta = 1/2 + \sum_{\alpha=x,y,z}(\lambda_\alpha)^{-1}$ and $\zeta(x)$ is Riemann zeta function. For the cases of a flatbottom box and

three-dimensional harmonic oscillator, η is equal to $1/2$ and 2, respectively, leading to

$$\text{3D box:} \quad s_t^\star = \frac{5\zeta(5/2)}{2\zeta(3/2)} = 1.284\ldots$$
$$\text{3D HO:} \quad s_t^\star = \frac{4\zeta(4)}{\zeta(3)} = 3.602\ldots. \tag{23}$$

Finally, assuming the trap has a positive fixed-N heat capacity, $C_N = \frac{\partial}{\partial T}|_N E = T\frac{\partial}{\partial T}|_N S > 0$ and the critical number of particles monotonically increases with temperature, $\frac{\partial}{\partial T} N^\star > 0$, one can show that the BEC condition (20) is equivalent to the following condition on the entropy per particle:

$$s_t \le s_t^\star \Longleftrightarrow \text{BEC}. \tag{24}$$

This form of the BEC criterion is particularly useful for analysis of adiabatic processes.

Lattice-to-trap transfer process.—Consider the following process. First, atoms are loaded into the optical lattice and thermalized. Next, an external trap is built around the lattice. Finally, the original lattice is removed, and the state of the resulting gas is detected. The process is schematically depicted at Fig. 1.

The transfer from lattice to trap is assumed to be thermodynamically adiabatic, and therefore the entropy of the system is conserved throughout the process. In particular, the entropies of the final trap and original lattice must be the same: $S_t = S_l$. Since the number of particles N is also conserved, the above conservation law can be reformulated as

$$s_t = s_l, \tag{25}$$

where $s = S/N$ is the entropy per particle. Consider a two-dimensional plane whose coordinates are given by the peak lattice site occupation $\bar{n}$ and ground state fraction in the occupied sites w_0. The no-BEC vs BEC transition line in this plane will be thus given by an implicit equation,

$$s_l(\bar{n}, w_0) = s_t^\star, \tag{26}$$

where $s_l(\bar{n}, w_0)$ is the entropy per particle in the original lattice, and $s_t^\star$ is the critical entropy per particle for the given trap.

The gas in the final trap will (not) be a BEC if the lattice entropy is below (above) the critical value $s_t^\star$. The lattice and critical trap entropies were explicitly computed above for two particular cases each. The four resulting phase diagrams are shown in Figs. 2 and 3.

In a harmonic trap, the peak phase-space density exceeds the average phase-space density. Because the peak phase-space density determines the BEC threshold [14], BEC is more readily obtained when lattice atoms are transferred to a harmonic trap than to a flatbottom trap [compare Figs. 2(b) and 3(b) to 2(a) and 3(a)]. When the initial distribution in the lattice is flat [Figs. 2(a) and 2(b)], the

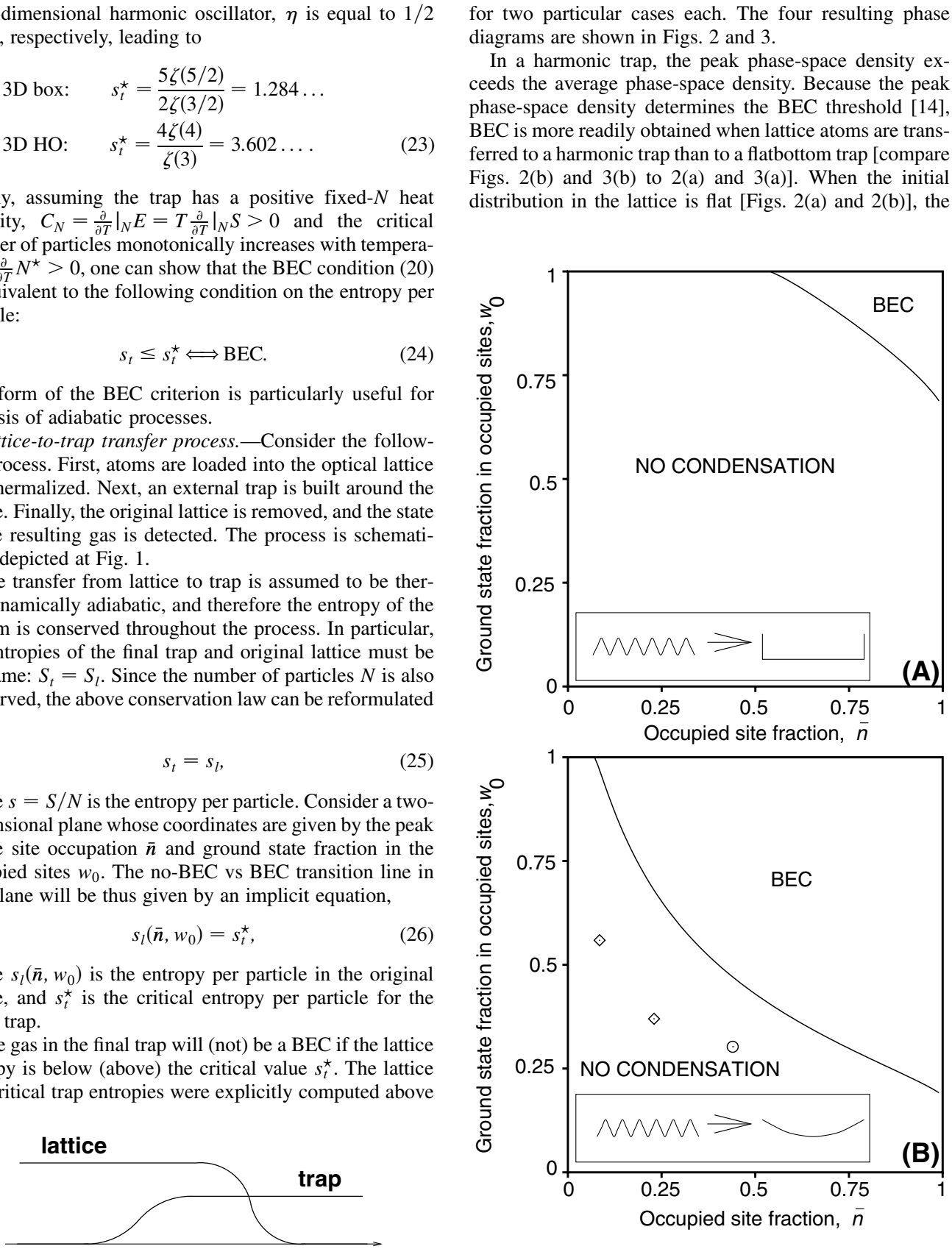

FIG. 1. An artist's view of the lattice-to-trap adiabatic transfer process.

FIG. 2. Phase diagram for flat-lattice-to-trap adiabatic transfer. The final traps are (a) flatbottom box and (b) 3D spherically symmetric harmonic oscillator. The experimental points correspond to results in Refs. [8] (circle) and [10] (diamonds).

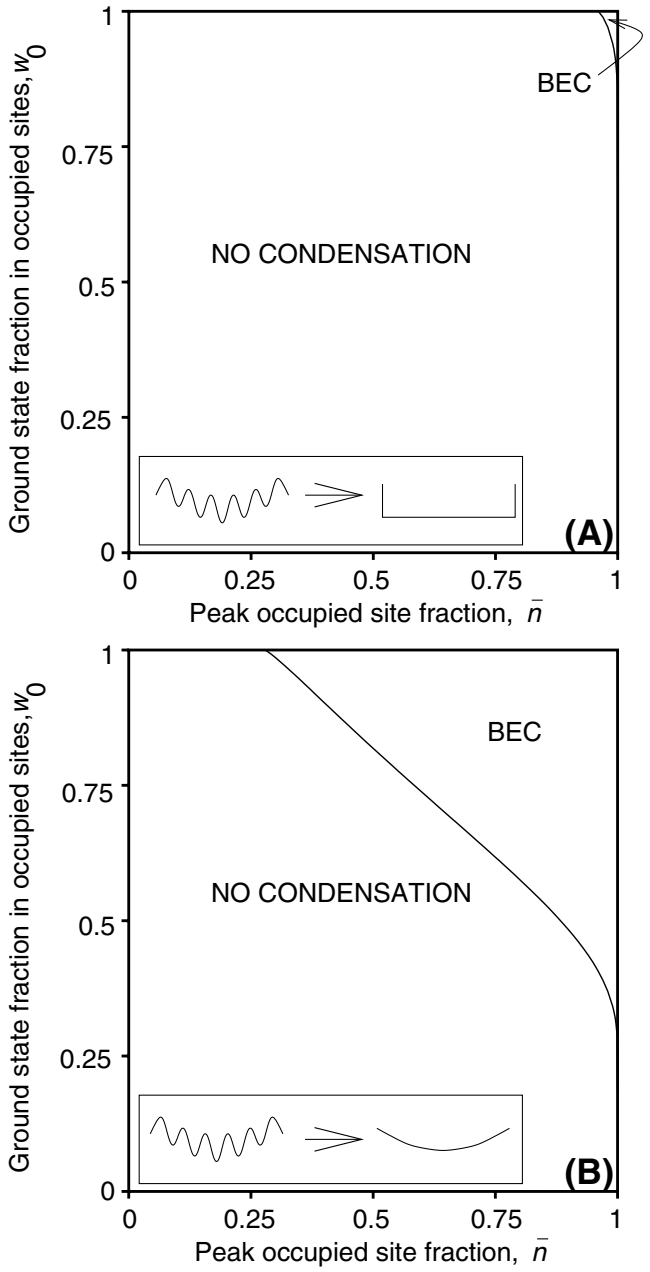

FIG. 3. Phase diagram for harmonic-lattice-to-trap adiabatic transfer. The final traps are (a) flatbottom box and (b) 3D spherically symmetric harmonic oscillator.

initial bulk phase-space density is constant across the sample. There is then more to be gained by changing the bulk shape of the trap than when the initial phase-space density is already nonuniform [Figs. 3(a) and 3(b)]. The combination of these effects qualitatively explains why the flat-lattice to harmonic trap scenario is the most promising approach to BEC [Fig. 2(b)].

Fortunately, the photoassociative collisions that limit the average site occupation to one half also flatten the large scale distribution [8]. Existing techniques can probably produce transient site occupations of several, which will naturally lead to approximately flattop distributions after laser cooling. Some published experimental results for laser cooling in 3D optical lattices are marked on Fig. 2(b). Further increases in the ground state occupation are feasible [10], especially by scattering light in the regime where the heating from rescattered photons is minimized [15]. As illustrated in Fig. 2(b), only a modest improvement is required to pass the BEC threshold.

In summary, we have related the entropy of atoms distributed in optical lattices to the entropy of atoms in harmonic and flatbottom traps. By entropy comparison, we have calculated BEC phase diagrams for lattice-bound atoms. These diagrams create a framework for considering experiments with BECs in optical lattices and suggest a way to obtain BEC without evaporative cooling.

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