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We investigate the effects of finite temperature on ultracold Bose atoms confined in an optical lattice plus a parabolic potential in the Mott insulator state. In particular, we analyze the temperature dependence of the density distribution of atomic pairs in the lattice, by means of exact Monte-Carlo simulations. We introduce a simple model that quantitatively accounts for the computed pair density distributions at low enough temperatures. We suggest that the temperature dependence of the atomic pair statistics may be used to estimate the system's temperature at energies of the order of the atoms' interaction energy.

I. INTRODUCTION

Great progress has been achieved in the coherent control and manipulation of ultracold atoms and molecules. In a series of recent experiments, several groups were able to demonstrate the loading of an atomic Bose-Einstein condensate into the lowest vibrational level of single wells of an optical lattice [1, 2, 3, 4, 5]. In a remarkable experiment, M. Greiner *et al.*, [1], demonstrated the capability of inducing a reversible quantum phase transition between a superfluid and an insulator state for bosonic atoms by varying the intensity of the trapping laser beams and therefore the depth of single potential wells. In a series of recent experiments, the same group demonstrated the capability of creating an array of quasi one dimensional tubes and induce an effective one dimensional superfluid/insulator transition, with on-site peak density equal to one [6, 7, 8]. Several proposals suggest this system has potentially fundamental applications in the field of quantum computation, as the realized array of atoms in the insulating regime can be used to create an ideal register for qubits [9, 10, 11, 12, 13].

A key observable in experiments with ultracold atoms is the interference pattern observed after a certain time of flight following the release of atoms from all trapping potentials. The interference pattern is proportional to the distribution of atomic momenta [14, 15, 16, 17], and provides direct information on the amount of phase coherence present in the system. Information extracted from the interference pattern is routinely used to measure the system temperature in the superfluid regime, but cannot be easily used in the strongly interacting regime, where both finite temperature and interactions compete to fill up the single-particle Brillouin zone. In fact, in time-of-flight images the measurement precision is on the order of the level spacing to the second lattice band, while the relevant energy scales in the strongly interacting regime are the onsite interaction energy and the hopping amplitude. The latter are typically at least one order of magnitude smaller than the lattice level spacing [18]. Thus, apart of a scheme based on fermionization of the many-body wavefunction [6], to date there are no available schemes for the estimation of temperature at energies of the order of the interaction energy in the strongly correlated regime.

Recently, time-of-flight images have provided evidence for the mixing of particle-hole excitations in the ground state in the Mott regime Ref. [7, 8]. This mixing has important consequences for the use of the Mott state as a quantum register. In fact, the presence of empty and doubly occupied sites introduces unwanted errors in the register initialization, which have to be corrected for at the cost of overheads in computational resources and gate times. A characterization of the finite-temperature population of particle-hole states in realistic experimental conditions is thus desirable.

In this work we analyze the effects of finite temperature on the Mott insulator state in the presence of an external parabolic potential. We focus on the effects of temperature on the density distribution of doubly occupied sites, showing that at finite temperature the latter has a characteristic site-dependent Gaussian profile due to the presence of the external potential. We derive the functional form of this temperature dependence by introducing an effective single-particle model for the many-body spectrum at energies of the order of the interaction energy, and we compare our model's predictions for the atomic pair density distribution to exact quantum Monte-Carlo results for realistic experimental parameters of the trapping potentials, finding good agreement. We suggest that the temperature dependence of the density distribution of doubly occupied sites may be used to estimate the system's temperature at energies of the order of the interaction energy.

The presentation of the results is organized as follows. In Sec. II we review the physics of the Mott insulator state and the low-energy spectrum of the Bose-Hubbard Hamiltonian both in homogeneous and inhomogeneous lattices. In Sec. III we introduce an effective model for the many-body spectrum at energies of the order of the interaction energy, and provide an analytical expression for the temperature dependence of the density distribution of atomic pairs at low enough temperatures. In Sec. IV we validate our model by comparing the analytical results to exact quantum Monte-Carlo simulations. In Sec. V we address the stability of the Mott insulator state against finite temperature population of particle-hole states. In Sec. VI we discuss the possibility of estimating the system's temperature by collecting statistics of the presence of atomic pairs in the lattice. Finally, the conclusions are presented in Sec. VII.

II. THE MOTT INSULATOR STATE

The Bose-Hubbard Hamiltonian describes the system's dynamics when the lattice is loaded such that only the lowest vibrational level of each lattice site is occupied [18]

$$H_{BH} = \sum_j \left[\epsilon(j) n_j - J(a_j^\dagger a_{j+1} + a_{j+1}^\dagger a_j) + \frac{U}{2} n_j(n_j - 1) \right]. \quad (1)$$

Here a_j is the bosonic annihilation operator of a particle at site j and $n_j = a_j^\dagger a_j$. The site-dependent $\epsilon(j)$ models an external magnetic quadratic potential, while J and U are the tunneling and on-site interaction energies respectively. For deep lattices with potential energy $V(x) = V cos^2(kx)$, the tunneling energy is approximated by $J = 4/(\sqrt{\pi}) E_R (V/E_R)^{3/4} e^{-2\sqrt{V/E_R}}$, where $E_R = (\hbar k)^2/2m$ is the recoil energy, k the light wave vector, and m the atomic mass. The on-site interaction energy is due to ground state collisions between atoms each in the motional state $\phi(\mathbf{x})$ and is given by $U = \frac{4\pi a_s \hbar^2}{m} \int d\mathbf{x} |\phi(\mathbf{x})|^4$, with a_s the s-wave scattering length and $\phi(\mathbf{x})$ a Wannier state. J and U are assumed to be site independent [18].

For a homogeneous one dimensional lattice ($\epsilon(j) = 0, \forall j$) of M sites with periodic boundary conditions at zero temperature T, an insulating state, the *Mott state*, occurs only if the number of particles N equals M and the interaction energy dominates over the tunneling energy. If $\sqrt{N} J/U \ll 1$ the ground state has approximately energy $E_g = -4NJ^2/U$ and is given by

$$|\Psi_g\rangle = \alpha(|T\rangle + 2\sqrt{N} J/U |S\rangle), \quad (2)$$

where the normalization constant is $\alpha = (1 + 4N(J/U)^2)^{-1/2}$. The Fock state $|T\rangle = \Pi_{j=1}^N a_j^\dagger |0\rangle$ has one particle per site and zero energy, and the symmetrized state $|S\rangle = 1/\sqrt{2N} \sum_{j=1}^N (a_j^\dagger a_{j+1} + a_{j+1}^\dagger a_j)|T\rangle$ has energy U. Indeed, in the homogeneous system all Fock states with an empty site and an atomic pair in another site are degenerate with energy U. The latter is roughly the lowest excitation energy for the many-body system in the homogenous commensurately filled case [19].

The probability of creating exactly $N = M$ particles in an experiment is negligible. An insulator state can be recovered if an external quadratic potential is present. Then, $\epsilon(j) = \Omega j^2$ where $\Omega = m(\pi/k)^2 \omega_T^2/2$ is a characteristic energy scale for a trap of frequency ω_T. At $T = 0$, a Mott state with average occupation one in the center of the trap can be realized for $\sqrt{N} J/U \ll 1$ if

$$N < M, \qquad U > \epsilon((N-1)/2), \qquad \Omega N > J. \quad (3)$$

The last two inequalities insure that multiple particle occupancy and tunneling of holes from the borders to the center of the lattice are suppressed, respectively [12]. The first inequality in Eq. 3 simply states the number of wells be larger than the number of atoms. As a consequence, there are $M!/((M-N)!N!)$ Fock states with maximal on-site occupation one, at variance with the single state of the case $N = M$. In the presence of the trap these states are not degenerate, spanning an energy range which may be larger than U. We redefine as $|T\rangle = \Pi_{j=-(N-1)/2}^{(N-1)/2} a_j^\dagger |0\rangle$ the lowest energy state and set its energy to zero [20]. The state $|T\rangle$ is the ground state of the system to zeroth order in J, while the true ground state has coherences due to tunneling of a hole in either one of sites $\pm(N-1)/2$ and mixing of Fock states $|S_{n,m}\rangle = a_n^\dagger a_m |T\rangle/\sqrt{2}$ with an atomic pair and a hole at sites n and m respectively, with $n, m < |(N-1)/2|$, in analogy to the homogeneous case. States $|S_{n,m}\rangle$ are not degenerate, due to the trap presence. States $|S_{n,m}\rangle$ with $m = n \pm 1$ dominate the mixing into the ground state, and for $\Omega \ll U$ the amplitude of mixing approaches the homogeneous system's one $\sqrt{2}\alpha J/U$.

In general, the $|T\rangle$-state is coupled *via* the BH-Hamiltonian to $|S_{n,m}\rangle$-states with a matrix element of order $(J/U)^{|n-m|}$, which is negligible for $|n-m|$ large enough in the insulating regime. On the other hand, a temperature of the order of the energy difference between $|T\rangle$ and $|S_{n,m}\rangle$-states allows for population of the latter. In particular, the lowest energy Fock state $|S_{n,m}\rangle$ has two particles in the central site of the lattice and a hole at site $|(N-1)/2|$. Its energy is $\tilde{\Delta} = U - \epsilon((N-1)/2)$. This state is an eigenstate of the BH-Hamiltonian for $J = 0$ only. For any finite J, eigenstates are a superposition of many different Fock states. This superposition lowers the energy $\tilde{\Delta}$ of an amount W which is of the order of a few J. As a consequence, the energy Δ of the lowest-energy eigenstate with two atoms in a site is reduced to approximately $\Delta = \tilde{\Delta} - W$. In the following we introduce a simple model for the spectrum of the many-body system at energies of order Δ, which we find to be the relevant energy scale for the double occupation of a site in the lattice [11].

III. EFFECTIVE SINGLE-PARTICLE SPECTRUM

Neglecting for a moment mixing of $|S_{n,m}\rangle$-states in low lying modes, we expect that the density distribution of atomic pairs as a function of the position in the lattice at finite temperature T has a a Gaussian profile for the following argument. Given a lattice with M wells, $N = M + 1$ particles and $U \gg J$, the ground state has roughly one particle per site and an extra particle at the center of the trap, forming an atomic pair. For weak enough quadratic traps, $\Omega \ll J$, tunneling of the extra particle is not suppressed over a certain number of lattice sites at the center of the trap where the external potential is essentially flat, meaning that the atomic pair acts approximately as a conventional harmonic oscillator with *effective* mass $m_* = 1/(4J)$ and trapping frequency $\omega_* = 2\sqrt{2\Omega J}$. Here the lattice constant $a = \pi/k$ and $\hbar = h/2\pi$ have been set to unity, where h is the Planck constant. The tight binding spectrum is therefore approximated by an harmonic oscillator spectrum whose level spacing is ω_* with an error of order $O(\Omega/J)$. If $T > \omega_*/k_B$, it can be shown that the quantum density distribution $P(j)$ for the atomic pair becomes equivalent to the classical distribution

which is proportional to

$$P(j) \propto e^{-\beta m_* \omega_*^2 j^2/2} = e^{-\beta\Omega j^2} \quad (4)$$

where $\beta = 1/(k_B T)$, and k_B is Boltzmann constant. The distribution $P(j)$ as a function of lattice site j, Eq. 4, is therefore a Gaussian whose width is $x_0 = \sqrt{1/(2\beta\Omega)}$.

We postulate that for realistic situations where $M > N$ harmonic oscillator states actually approximate the incomplete basis set defined on the central N sites of the lattice in the energy range $\Delta \lesssim E \ll 3U - 2\epsilon((N-1)/2)$, where $3U - 2\epsilon((N-1)/2)$ is a characteristic energy for population of states with three particles in one of the central $N-2$ sites. Apart of a normalization factor, we therefore expect that the density distribution as a function of the position j in the lattice has the same Gaussian profile as in Eq. 4 with an exponential suppression due to the energy shift Δ

$$P(j) \propto e^{-\beta\Delta} e^{-\beta\Omega j^2}. \quad (5)$$

The width x_0 of the density distribution can be therefore directly related to the temperature of the sample, for $k_B T \lesssim \Delta$. In fact, while for a temperature of order Δ states are populated with more than one pair in the central sites, the various pairs approximately behave like non-overlapping harmonic oscillators, meaning that the probability of finding two extra particles in the same site is strongly suppressed. Therefore, the density distribution at a single site should still approximately maintain a Gaussian profile of width x_0. Moreover, the height of the Gaussian peak is an indication of Δ, and therefore of the number of particles N. For vanishing values of J, Δ is approximately $\tilde{\Delta}$, and the peak's height is easily computed. For $J > 0$, the shift $W = \Delta - \tilde{\Delta}$ is of the order of half of the pair's band-width. Because the latter is $8J$, W is approximately $4J$. Because the peak's height also depends on the normalization, we expect Eq. 5 to well approximate the value of the density peak for $k_B T \ll \Delta$, where the normalization is almost one.

The modeling of the excited states of the many-body system with an effective harmonic oscillator spectrum for atomic pairs is one of the central results of this paper. In the following we verify the accuracy of this picture by comparing the model's predictions for the atomic pair density distribution to exact Monte-Carlo results.

IV. NUMERICAL SIMULATIONS

We perform numerical simulations of the density distribution of atomic pairs in the lattice as a function of temperature for some realistic experimental parameters. We employ a quantum Monte-Carlo code based on the continuous-time Worm algorithm [21]. A sample of $N = 101$ atoms of ^{87}Rb is trapped in a lattice with wavelength $\lambda = 785$ nm and parallel and transverse confinements $V_\parallel = 15E_R$ and $V_\perp = 40.5E_R$ respectively. Using $a_s = 5.6$ nm, the interaction energy in frequency units is $U/h = 3.340$ kHz and $U/J = 120$. The

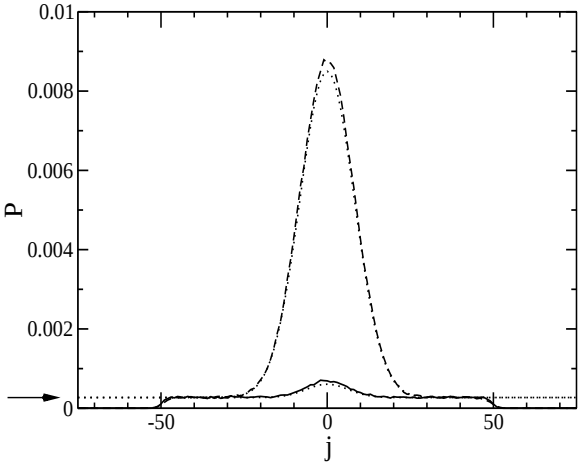

FIG. 1: Density distribution of atomic pairs P as a function of the lattice index j. Continuous and dashed lines are numerical results for $T = 3J/k_B$ and $T = 5J/k_B$ respectively. Dotted lines are analytical curves for the same temperatures. The arrow indicates the zero-temperature mixing of $|S_{n,n\pm1}\rangle$-states. Here $N = 101$, $U/J =$

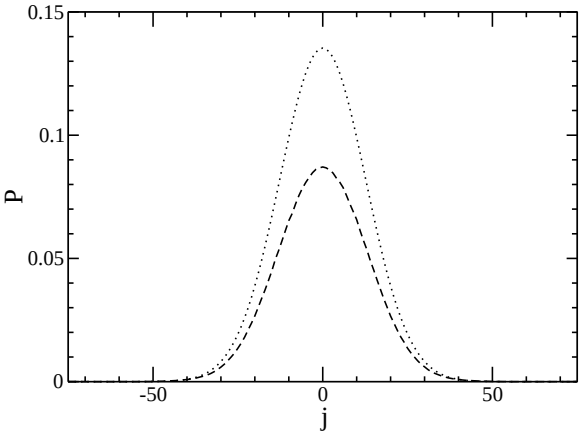

FIG. 2: Density distribution of atomic pairs P as a function of lattice index j, for $T = 12J/k_B$. Dashed and dotted lines are numerical and analytical results respectively. Here $N = 101$, $U/J = 120$, $\Omega/J = 0.0374226$, and $\Delta/J = 24$.

external magnetic trapping frequency is $\omega_T \approx 2\pi \times 40$ Hz and therefore the number of atoms N fixes $\epsilon(N-1)/2 \approx 0.8U$, and thus $\Delta \approx 24J$. We have chosen these parameters because they are experimentally feasible and satisfy Eq. 3, so that at zero temperature a Mott state is formed with one particle occupying each one of the central N sites of the lattice. In particular, zero temperature mixing of basis states with an empty site in one of the central N sites of the lattice is suppressed, the largest amplitude of mixing corresponding to the outer most trapped particle tunneling to the adjacent empty site. Calculations have been performed for $M \gg N$, so that atoms never reach the border of the lattice. We note that $N = 101$ compares well with the typical number of atoms present in

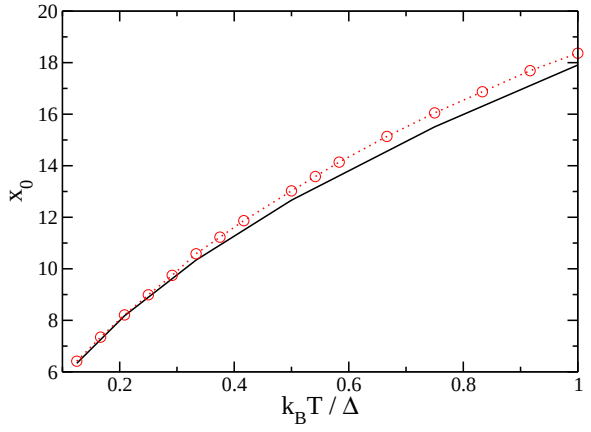

FIG. 3: (Color online) Width x_0 of the density distribution of atomic pairs as a function of k_BT/Δ. The width x_0 is in units of the lattice constant a. Circles(red) are numerical values, while the continuous line is the analytic curve $(k_BT/2\Omega)^{1/2}$. Here $N = 101$, $U/J = 120$, $\Omega/J = 0.0374226$, and $\Delta/J = 24$.

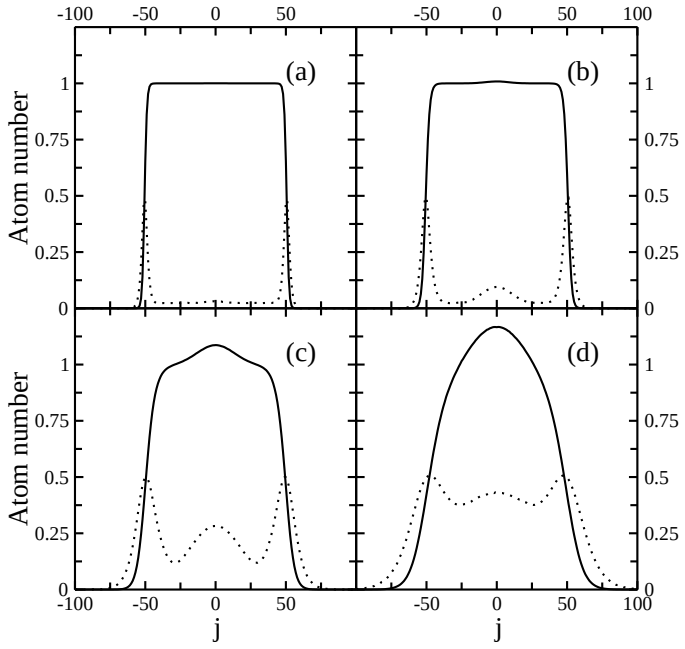

FIG. 4: Local densities and fluctuations as a function of the site index j for $k_BT/J = 3(a), 5(b), 12(c)$, and $24(d)$. Here, $\Delta/J = 24$. Continuous and dotted lines are the numerical densities and fluctuations, respectively.

the one-dimensional tubes of Refs. [2, 3, 4, 5, 6, 7, 8]. For example, N is equal to 80 in the central tube of Ref. [5], which is the largest number of atoms for the entire array of tubes, while N is as small as 20 in the central tube of Ref. [6] .

In Fig. 1 the atomic pair density distribution P is plotted as a function of the site index j for $Tk_B/J = 3$ and 5. Continuous and dashed lines are numerical results, while dotted lines are analytical curves. For $Tk_B/J = 3$, lower curves, the numerical solution shows essentially a flat density distribution throughout the central N sites, with a shallow gaussian peak at the center. The flat distribution corresponds to the zero temperature residual mixing of $|S_{n,n\pm1}\rangle$-states into the ground state, characteristics of the Mott state. The results of Ref. [7] are consistent with the observation of this mixing. As $\Omega \ll U$, corrections to the density distribution due to the external trapping potential are not distinguishable on the scale of the graph, and the on-site density matches the homogeneous system's value $2 \times 2(J/U)^2 \approx 0.000278$. The factor of two in front of last expression is due to the fact that the extra atom can tunnel from the left or right. The latter constant has been added to the analytic curves, and is indicated by an arrow in Fig. 1. Finite atomic pair density due to zero-temperature mixing of $|S_{n,n\pm1}\rangle$-states is a direct signature of the creation of a Mott state. For sufficiently low temperatures, selective probe of the density distribution in lattice sites j with $j \gg x_0$ can give direct *in situ* evidence of the formation of the Mott plateau in the center of the trap, while the shallow peak around $j = 0$ measures finite temperature population of $|S_{n,m}\rangle$-states.

For $Tk_B/J = 5$ the Gaussian peak is more evident on the scale of the graph. We observe that numerical and analytical curves nearly overlap. In particular, the widths of the Gaussians perfectly match, while the height of the peak is slightly underestimated by the analytic curve. This is due to the fact that Δ is only approximately $24J$ for the chosen parameters, and the difference is amplified by the exponential function. A larger disagreement in the peak height is observable for $k_BT/J = 12$ in Fig. 2, where the analytic curve largely overestimates the exact result. This is expected, as for higher temperatures the normalization constant differs more and more from one, therefore suppressing the peak height in the exact solution.

In Fig. 3 the width x_0 is plotted against the temperature, up to $T = \Delta/k_B$. Circles are numerical results, while the continuous line is the analytic solution $\sqrt{k_BT/(2\Omega)}$. The plot shows an almost perfect agreement between numerical and analytical results for $k_BT \lesssim \Delta/4$. Deviation for higher temperatures is due to population of states with a large number of atomic pairs. For $k_BT = \Delta$ the deviation is still less than a lattice constant. We consider the good agreement between the analytic model and the numerical results over the entire range $k_BT \leq \Delta$ as a strong indication of the validity of the harmonic oscillator model.

V. FINITE-T DEPLETION OF THE MOTT STATE

A large population of states with two particles in a site will ultimately totally deplete the Mott state, thus making any application of the Mott insulator state to quantum computation schemes impossible. In the remainder of this section we investigate the role of the energy scale Δ in the thermal depletion of the Mott insulator state, by numerically analyzing the atomic

density profile and onsite number fluctuations.

In Fig. 4 the on-site atomic density $\langle n_j \rangle$ (continuous lines) and the number fluctuations $\langle \Delta n_j \rangle = \sqrt{\langle n_j^2 \rangle - \langle n_j \rangle^2}$ (dotted lines) are plotted as a function of the site index j, for $k_B T/J = 3(a), 5(b), 12(c)$, and $24(d)$. For $k_B T/J = 3$ the density profile is flat, which corresponds to an extended Mott state around $j = 0$. The number fluctuations are also flat throughout the lattice, except for two large peaks around $\pm N/2$ and a small bump at the trap center. The flat regions correspond to the zero-temperature mixing of particle-hole states [16, 22], which is approximately given by $2\sqrt{2}J/U$, while the large peaks are due to the tunneling of particles to unoccupied sites, and are equal to ΩN [16, 22]. The small bump at the trap center corresponds to the finite-temperature population of high-energy states with two particles in a site, analogous to the discussion of Fig. 1. Panels (b) and (c) show that for higher temperatures atoms tend to accumulate at the trap center, therefore decreasing the extension of the region of constant density. For $k_B T = 24J = \Delta$ the Mott state has completely disappeared.

In Ref. [23] the effects of finite temperature on the stability of the Mott insulator state have been studied by means of classical Monte-Carlo simulations, finding that well defined Mott insulating plateaux are present for temperatures at most of the order of $U/(10k_B)$. The discussion above shows that, for any fixed U and Ω, this is true only in the limit of a small number of particles N. In fact, we showed that the relevant energy scale for population of doubly occupied site is $\Delta = U - \Omega((N-1)/2)^2$, which is N-dependent. In particular, for a system with $N = 110$ instead of $N = 101$, we have $\Delta \approx 9J$. In this case, a temperature of the order of $U/(10k_B) = 12J/k_B$ would be larger than Δ and would therefore completely deplete the Mott insulator state.

VI. TEMPERATURE ESTIMATION

As mentioned above, it is notoriously difficult to measure temperatures of the order of the interaction energy in the strongly interacting limit.

On the other hand, we have shown above that the atomic pair density distribution has a clear temperature dependence. Here we suggest that in principle this temperature dependence may be used to estimate the system's temperature at energies of the order of Δ, by devising a probe that is sensitive to the presence of multiply occupied sites in the lattice. For this purpose, two different kinds of experiments may be considered. The first possibility is to design an experiment which is solely sensitive to the total number of pairs in the lattice. The latter can be calculated numerically as a function of temperature by means of quantum Monte-Carlo simulations, and the results of the simulations can then be compared to the experimental data to extract a temperature estimation. An example of these calculations for the trapping parameters given above and $N = N_{tot} = 101$ is given in Fig. 5, where the total number of pairs N_2 is plotted as a function of the temperature. In the plot, the circles (red) are the quantum Monte-Carlo results for $N_{tot} = 101$, while the squares (blue) and the diamonds (green) correspond to a total number of particles $N_{tot} = 95$, and 107, respectively. Each curve is normalized to $N = 101$. The curves for $N_{tot} = 95, 107$ are shown in order to take into account a plausible experimental uncertainty on the total number of atoms N_{tot}. In fact, it is experimentally challenging to control the total number of particles N_{tot} to better than 5 percent, and the uncertainty on the total number of particles is likely to dominate the experimental errors [24]. Then, assuming unit efficiency of atomic pair detection, for each measured N_2 the temperature is easily estimated. For example, for the system considered above, where $N_{tot} = 101$, if 5 pairs ($N_2/N \approx 0.04$) are measured experimentally, a simple analysis of Fig. 5 yields a most-probable temperature of about 14.4 J/k_B (0.6 Δ/k_B). Thus, by taking into account the uncertainty on the total number of atoms (black-dashed line in the plot), the final estimate for the temperature is $T = (14.4 \pm 4.0)J/k_B$.

We note that the discussion above refers to the determination of temperature in a single experiment. If one wants to determine average system's temperatures, the measurement can be repeated many times, and the error bars are obtained by assuming a shot-to-shot Poissonian fluctuation of N_{tot}, in analogy to the discussion above. However, in the remainder of this section we discuss an experiment that allows for the estimation of average system's temperatures and it is largely independent of the fluctuations of N_{tot} (although it is admittedly difficult to implement).

In principle various schemes may be used to experimentally detect the presence of pairs in the lattice. Here, we propose to collect statistics of atomic pairs through resonant photo-association of two atoms in a single well to a molecular excited state, followed by ionization of the formed molecules and detection of the emitted ions. In fact the latter can be performed with almost unit efficiency [24]. For this experiment. the molecular excited state should be chosen

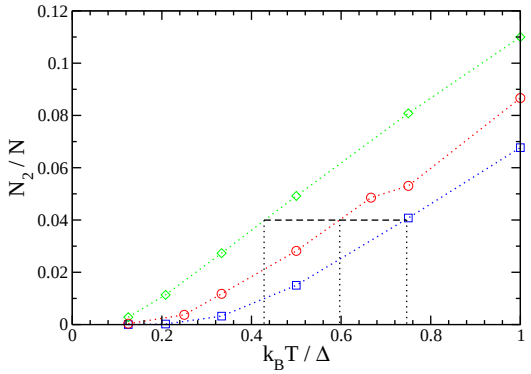

FIG. 5: (Color online) Number of atomic pairs N_2 as a function of $k_B T/\Delta$. Here, N_2 is in units of $N = 101$. The squares(blue), circles(red), and diamonds(green) correspond to systems with $N_{tot} = 95, 101$, and 107 atoms, respectively. For all curves, $\Delta/J = 24$. The dashed line is the error bar for the temperature estimation, given a measured number of pairs equal to 5 ($N_2/N \approx 0.04$). The dotted lines are a guide to the eye.

to be far from atomic dissociation, meaning that the atomic probability of spontaneous emission is not enhanced by the photo-associative laser.

The second kind of experiment that may be envisioned is one where the probe has a high spatial resolution, so that it is possible to determine the position of the atomic pair in the lattice. In this case, information on average system's temperatures may be extracted by measuring the width x_0, which has been shown above to depend only on the temperature and the known trap geometry. The advantage of this experiment is that x_0 is insensitive to N_{tot}. Thus, calibration of average system's temperatures may be performed by accumulating statistics of pair detection on successive experiments with the same trapping potentials, without worrying about possible fluctuations of N_{tot} from one experiment to the next.

Although a careful discussion of the sources of uncertainty on the measurements is out of the scope of the present analysis, we expect that a significant uncertainty on the temperature measurement is likely to come from the finite spatial resolution of the probe-field. In fact, for typical experimental setups it is not possible to focus a photo-associative laser onto a single site. The intensity of the photo-associative laser has a Gaussian profile whose width σ_L is typically of the order of the light's wavelength or larger. This means that the laser intensity may not be negligible on a few lattice sites, depending on the ratio between the wavelength of the photo-associative laser and the lattice constant a. A convolution between the pair density-distribution Gaussian and the laser-intensity Gaussian provides an estimate of the experimentally measured width x_0', which is thus given by $x_0' = \sqrt{x_0^2 + \sigma_L^2}$. We note that the difference between x_0 and x_0' decreases with increasing temperature. For example, for a reasonable value $\sigma_L = 3a$, $x_0' - x_0$ is approximately $0.6\ a$ for $k_B T = 0.2\Delta$, while it drops to $x_0' - x_0 \approx 0.3a$ for $k_B T = 0.6\Delta$.

Finally, we note that it is straightforward to generalize the calculations above for the array of one-dimensional tubes of Refs. [2, 3, 4, 5, 6, 7, 8]. Assuming an initial Thomas-Fermi distribution of the atoms in the three dimensional system, the calculations above may be repeated for each tube separately and the results combined (see also Ref. [6]).

VII. CONCLUSIONS

In summary, we have studied the effects of temperature on the Mott insulator state, with an emphasis on the finite temperature population of states with two atoms in a site. We introduced a model for the energy spectrum of the trapped many-body system in the strongly correlated regime, which allowed us to derive the functional form of the dependence of the density of atomic pairs upon temperature. We discussed the depletion of the Mott state due to the population of states with multiple on-site occupancy. Finally, we suggested that the temperature dependence of the density distribution of doubly occupied sites may be used to estimate the system's temperature at energies of the order of the interaction energy.

Note added: After this work was completed, the results of an experiment analogous to one of those proposed here have been presented in Ref. [25], where the temperature of a fermionic Mott state has been estimated.

VIII. ACKNOWLEDGEMENTS

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