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A THEORETICAL METHOD OF EVALUATION OF TOTAL MOMENTUM DISTRIBUTION N(K), CONDENSATE MOMENTUM DISTRIBUTION N_0(K) AND NON-CONDENSATE MOMENTUM DISTRIBUTION N_{NC}(K) AS A FUNCTION OF K(Π/A) USING BOSE-HUBBARD MODEL

JITENDRA KUMAR SINGH[2], L. K. MISHRA[1]

1. Department of Physics, Magadh University, Bodh-Gaya-824234 (Bihar)
2. Department of Physics, Alma Iqbal College, Biharsarif, Nalanda (Bihar)

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Abstract: - Using the theoretical formalism of **U. Ray and D. M. Ceperley (arXiv;1209.1053v2(2012)),** we have studied condensate and non condensate spatial and momentum distribution in Bose-Hubbard model. We have also theoretically estimated spatial and momentum distribution of condensate and non condensate in far field ($r \to \infty$) and for finite TOF (Time of flight)(τ=20ms) as a function of k(π/a). Our theoretically evaluated results indicate that one can calculate exact n_0 and used to characterize and study phase transition. Our theoretically evaluated results are in good agreement with other theoretical workers.

Keywords: Condensate and non condensate momentum distribution, Optical lattice experiment (OLE), Time of flight (TOF) measurements, Hartree-Fock-Bogoliubov-Popov Approximation, Quantum Monte Carlo (QMC) technique, Local density approximation (LDA), Quantum depeletion (QD), Analytical MFT method, Mott insulating (MI) phases, Column integrated momentum distributions

Corresponding Author: MR. JITENDRA KUMAR SINGH

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INTRODUCTION

The physics of Bose-Einstein condensation particularly magnetically trapped Bose gases has strongly correlated phases because of low particle density. It has been proposed that one can exploit the strong interactions that are available in systems of Bose atoms confined in an optical lattice[1]. The Bose-Hubbard model[2] has been the focus of intensive research for strongly correlated phases. This model was realized basically with cold atoms in optical lattice. Optical lattice experiments (OLE) are prime candidate for quantum simulations due to their extensive tenability and control. They serve as ideal system to study dynamical phenomena of many body effects in strongly interacting systems. In this study the systematic characterization of equilibrium properties are crucial. The important quantities are temperature and density. The direct measurement of temperature is OLE which is an area of active research[3,4]. Further the study of phase transition requires a good understanding of an observable that can be used as a probe for the state of the system. Theoretically the natural choice is the order parameter and for B-H model is the condensate fraction $n_0=N_0/N$, where N_0 is the total number of condensed atoms and N is the number of atoms.Alternatively[5,6] super fluid fraction characterizes the transition but this is not simple to measure in cold atoms systems. The most easily accessible observables in experiments are the entropy and n_0 that comes from time of flight (TOF) measurements. The entropy is measured from TOF measurements while the atoms are in harmonic trap and n_0 is measured directly from TOF expansion after all field are "snapped off ''. The n_0 is useful since combined with entropy is used for thermometry in experiments[7].

In homogeneous systems, n_0 is given by delta function at the origin in momentum space. But in the case of inhomogeneous systems, n_0 is no longer simply given by the occupation number at zero momentum. One generally handle the trap in the mean field theory (MF) with Hartee-Fock-Bogoliubov-Popov approximation[8,9] for small interaction strength U or the site-decoupled approach for large U. One also uses local density approximation (LDA)[10]. In situation where MF result no longer match with the experimental data, one can use exact Quantum Monte Carlo(QMC) technique. Generally Quantum Monte Carlo (QMC) has been used to directly compare observable with measurements. But order parameter has not been computed and compared directly with experiments. Here, one adopts a approach in which experimental TOF images are taken and fit to obtain the number of condensed atoms under the peak and also number of non-condensed atoms. The ratio of the former to the sum of two is defined as the peak weight[6] or the coherence fraction[3] f_0 that serves as proxy of n_0. In earlier experiments, thermometry was done by comparing full momentum distributions together with f_0, peak width w_0 and visibility directly to QMC results. The last three observables were further used to characterize the critical temperature T_C for transition from normal to super fluid phase. Unfortunately these probes are not necessarily reliable estimates of the order parameters since the relation between n_0 and f_0 is not well understood. Previous measurements show large differences. In general, it was realized that n_0 is very good probe for phase transitions and it is also indicative of the effect of the interactions i.e. quantum depletion (QD) combined with the entropy measurements n_0 would be an excellent probe for T.

In this paper, using the theoretical formalism of U. Ray and D. M. Ceperley[11], we have evaluated the condensate and non-condensate momentum distributions using Bose-Hubbard model. We have evaluated total momentum distribution n(k), condensate momentum distribution $n_0(k)$, and non-condensate momentum distribution $n_{nc}(k)$ as a function of k(π/a) for Far field ($r \to \infty$) and also for finite TOF (τ=20ms). Our theoretically evaluated results are in good agreement with the experimental data and also with other theoretical workers[12,13].

MATERIALS AND METHODS

One starts with the Bose-Hubbard Hamiltonian (B-H)

$$H = -t\sum_{ij} a^{+}{}_{i} a_{i} + \frac{U}{2}\sum_{i} n_{i}(n_{i}-1) - \sum_{i}\mu_{i} n_{i} \tag{1}$$

Where t is the hopping integral between nearest neighbor sites i and j, $a_i^+(a_i)$ is Boson creation (annihilation) operator, $n_i=a_i^+a_i$ is the number operator and U is the on-site repulsive interaction.

$$\mu_i = \mu - V\left(\frac{r_i}{a}\right)^2 \tag{2}$$

This includes both the chemical potential with lattice spacing a where V is given by

$$V = \frac{1}{2}m\omega^2 \tag{3}$$

V is the curvature that is given by mass m and trapping frequency ω. Energy is given in atomic recoil energy units. E_r=167nK for ^{87}Rb and λ=800nm. The energy is used to create lattice. Lattices are taken between 70^3-100^3 with open boundary conditions.

One calculates the single particle density matrix $\widehat{\rho}_1(i,j)=\langle a^+{}_i a_i\rangle$ using stochastic series expansion and directed loop update algorithm. One defines the occupation of single particle states

$$\widehat{\rho}_1|\psi_i\rangle = N_i|\psi_i\rangle \quad (4)$$

Where the largest eigen value N_0 of $\widehat{\rho}_1$ gives the number of condensed atoms and $|\psi_0\rangle$ is the condensed wave function. The number of non-condensate atoms is given by

$$N_{nc}=\sum_{i\neq 0} N_i = N - N_0 \quad (5)$$

Here condensate is not fragmented and occupies only one mode in these systems, one uses iterative diagonalization procedure to obtain the spatial condensate wave function $\psi_0(r)$ and condensate momentum $\phi_0(k)$ is defined as

$$\phi_0(k)= F\,|\psi_0(r)\rangle \quad (6)$$

Where F is the Fourier transform[14]. The spatial non-condensate distribution is given by

$$n_{nc}(r)=n(r)-N_0|\psi_0(r)|^2 \quad (7)$$

The total momentum distribution is given by

$$n(k)=|w(k)|^2\sum_{j,l} e^{ik.(j-l)}\rho(i,j)$$

$$=n_0(k)+\sum_{p=1} n_p(k) \quad (8)$$

Where $|w(k)|^2$ is the Wannier envelope from which one can go from BH model to continuum model. In equation (8) the last term on the rhs is the momentum non condensate distribution n_{nc} (K)

In order to match with experiments one includes finite TOF effects[15] a site dependent phase term in equation (8) which is given by

$$n_p^{\,r}(k) = |w(k)|^2 N_p \sum_{jl} e^{ik.(j-l)-i(\frac{m}{2\hbar\tau})(p^2-l)} \langle j|\psi_p\rangle\langle\psi_p|l\rangle \tag{9}$$

Where τ is the TOF time, m is the mass of the particle. One uses $n_0^{\tau}(k)$ to denote the finite TOF condensate and $n_{nc}^{\tau}(K)$ for the finite TOF non-condensate distributions.

At sufficiently low temperature $n_{nc}(r)$ shows the quantum depilated (QD) atoms excited from $\psi_0(r)$ by the interactions. At intermediate temperature both thermal and interactions effects will cause depletion of the condensate.

Generally one starts with a non-interacting (NI) systems of particle at T>0 with a condensate ($n_0^{ni}(r)$) and a thermal distribution ($n_0^{th}(r)$). If one turns on interactions then the macroscopic occupation of the condensate will change and ($n_0^{ni}(r)$) will redistribute and expel particle to form a new $n_0(r)$ and QD states.

The time scale for the condensate to reach the far field is given by

$$\tau_{ff} = R\xi(1-\frac{\xi}{2R}) \tag{10}$$

Where R is the radial extent and ξ is the width of the condensate and τ_{ff} is the time scale for the condensate to reach the far field. Broader structure is observable within the experimental resolution

$$\Delta k = (\frac{m\pi\lambda}{h\tau})(\frac{\Delta r}{a}) \tag{11}$$

Where λ is the wavelength of the optical lattice, τ is the expansion time, Δr is the resolution then one obtains Δk resolution.

RESULTS AND DISCUSSION

In this paper using the theoretical formalism of U. Ray and D. M. Ceperley[11], we have theoretically evaluated total spatial n(r), condensate spatial distribution $n_0(r)$, non condensate spatial distribution $n_{nc}(r)$ as a function of r/a taking two sets of parameters U/t=25, N=60,000 and ω=68.5Hz (ii) U/t=60, N=58,000 and ω=67.6Hz. In **table T1**, we have shown the total spatial distribution n(r), condensate spatial distribution $n_0(r)$ and non condensate spatial distribution $n_{nc}(r)$ as a function of r/a taking U/t=25, N=60,000, ω=68.5Hz, K_BT/t=2.456 and n_0=0.21. Our theoretical results show that spatial distribution decreases with r/a. It is highest for n(r) and lowest for n_0(r). Spatial distribution vanishes for r/a>40, which is the onset of Mott-Insulating (MI) phases. In **Table T2,** we have repeated the calculations of n(r), n_0(r) and n_{nc}(r) as a function of r/a keeping U/t=40, N=58,000, ω=67.6Hz, K_BT/t=1.960 and n_0=0.19. Here, the same trend has been noticed condensate spatial distribution is the lowest. In **table T3,** we have again repeated the calculation of n(r), n_0(r) and n_{nc}(r) as a function of r/a keeping U/t=25, N=60,000, ω=68.5Hz, K_B/T=0.98 and n_0=0.62. Here, we observed that n(r) is the largest while the values of n_0(r) is nearer to n_{nc}(r). n_0(r) merges with n(r) for some values of r/a. In **table T4,** we repeated the calculations of n(r), n_0(r) and n_{nc}(r) as a function of r/a keeping other sets of parameters U/t=60, N=58,000, ω=67.6Hz, K_B/T=0.98 and n_0=0.48. Here also similar trend was observed. From these four calculations, it was observed that form of the condensate changes as U/t increases. At constant T, with increasing U/t the central occupation for the condensate continuously decreases until in the Mott Insulating (MI) phase it vanishes. The shape of n_0(r) changes with T because of mixing of states . Unlike non interacting (NI) problem, eigen states of the single particle Hamiltonian are not eigen states of ρ_1. It is also obvious that at colder temperatures, the condensate expands with more atoms at the edge of the trap rather than at the centre. This is because at the high density the centre leads to large possibilities of collisions and the condensate becomes saturated. Another interesting observation has been noticed due to U. Difference in shape of the condensate has been observed with different U but same n_0.

In **table T5,** we have shown the evaluated results of the Column integrated momentum distributions in the far field ($r \to \infty$). Here, we have shown the total momentum distribution n(k), condensate momentum distribution n_0(k) and non condensate momentum distribution n_{nc}(k) as a function of k(π/a). Others parameters are same as in table T1. We observed that all three n(k), n_0(k) and n_{nc}(k) show a peak at about k(π/a) =0. The values of n(k) and n_0(k) are almost same but n_{nc}(k) values lower than these two. In **table T6,** we repeated the calculation keeping other parameters same as in table T2 but the same trend is observed. In **table T7** and **tableT8,** we repeated the calculations changing other parameters as given in table T3 and Table T4 but the similar trend is observed. In all these four calculations, we observed the same features at any values of U/t. It is not just the shape of the condensate but rather all modes. It has also been observed that the peaks are formed around K= $\frac{2\pi}{\xi_0}$ where ξ_0 is the width of the condensate. This is because condensates are formed between boundaries (between the MI phase and the vacuum).

In **table T9 to tableT12,** we have shown the total momentum n(k), condensate momentum $n_0(k)$ and non condensate momentum $n_{nc}(k)$ as a function of k(π/a) for finite TOF(τ=20ms) keeping the values of others parameters same as in the previous calculations. We observed in all the four tables the values of n(k) and $n_0(k)$ are very much near to each other showing maximum value (peak) at k(π/a)=0 but the values of $n_{nc}(k)$ are different in all the four tables not only in values but also in shape. In table T9 and Table T10, $n_{nc}(k)$ show a peak at k(π/a)=0 but in table T11 and T12 its values are lowest at k(π/a)=0. It appears that for finite TOF effects alter the field distributions by suppressing central low k values. Furthermore, the functions with rapid spatial variations such as higher order modes of ρ_1 are not significantly affected by the site dependent phase shifts. Our theoretically evaluated results are in good agreement with other theoretical workers[12,13]. There is some recent results[15-20] which also reveals the similar behavior.

CONCLUSION

From the above theoretical analysis and investigations, we have come across the following conclusions

(1) We have studied the effects of interactions on the components of the spatial and momentum distributions of bosonic particles in a trapped optical lattice

(2) We have evaluated condensate and non condensate spatial and momentum distributions of the Bose-Hubbard model in a trap. We have studied the above distributions at far field ($r \to \infty$) and for finite TOF. We observe that both n (K) and $n^{\tau}(K)$ are broader for large U/t.

(3) We observed that the strong interactions cause condensate to develop a structure around the central peak very much like non condensate atoms.

Table T1: An evaluated result of total spatial distribution n(r), condensate distribution $n_0(r)$ and non-condensate distribution $n_{nc}(r)$ as a function of r/a keeping U/t=25, N=60,000, ω=68.5 Hz, K_BT/t=2.456 and n_0=0.21

r/a	n(r)	$n_0(r)$	$n_{nc}(r)$
0	1.000	0.326	0.784
5	0.925	0.308	0.722
10	0.834	0.267	0.686
12	0.746	0.245	0.635
15	0.682	0.220	0.597
20	0.605	0.208	0.532

22	0.584	0.187	0.486
25	0.476	0.138	0.392
30	0.358	0.087	0.305
32	0.273	0.053	0.216
35	0.186	0.023	0.164
40	0.054	0.007	0.072
45	0.023	0.002	0.005
50	0.006	0.000	0.000

Table T2: An evaluated result of total spatial distribution n(r), condensate distribution $n_0(r)$ and non-condensate distribution $n_{nc}(r)$ as a function of r/a keeping U/t=40, N=58,000, ω=67.6 Hz, K_BT/t=1.96 and n_0=0.19

r/a	n(r)	$n_0(r)$	$n_{nc}(r)$
0	1.000	0.000	1.000
5	0.925	0.000	0.936
10	0.806	0.158	0.812
12	0.763	0.266	0.774
15	0.709	0.355	0.696
20	0.654	0.446	0.634
22	0.608	0.503	0.595
25	0.532	0.425	0.528
30	0.486	0.328	0.446
32	0.354	0.263	0.375
35	0.262	0.205	0.306
40	0.198	0.116	0.215
45	0.146	0.074	0.138
50	0.066	0.008	0.034

TableT3: An evaluated result of total spatial distribution n(r), condensate distribution $n_0(r)$ and non-condensate distribution $n_{nc}(r)$ as a function of r/a keeping U/t=25, N=60,000, ω=68.5 Hz, K_B/t=0.98 and n_0=0.62

r/a	n(r)	$n_0(r)$	$n_{nc}(r)$
0	1.000	0.422	0.620
5	0.905	0.408	0.604
10	0.826	0.435	0.585
12	0.745	0.468	0.509

15	0.684	0.512	0.414
20	0.626	0.436	0.365
22	0.402	0.384	0.287
25	0.325	0.300	0.205
30	0.245	0.225	0.164
32	0.205	0.175	0.115
35	0.165	0.119	0.065
40	0.106	0.087	0.029
45	0.085	0.023	0.007
50	0.009	0.000	0.000

Table T4: An evaluated result of total spatial distribution n(r), condensate distribution $n_0(r)$ and non-condensate distribution $n_{nc}(r)$ as a function of r/a keeping U/t=40, N=58,000, ω=68.5 Hz, K_B/t=0.98 and n_0=0.48

r/a	n(r)	$n_0(r)$	$n_{nc}(r)$
0	1.000	0.002	1.000
5	0.952	0.056	0.965
10	0.916	0.124	0.922
12	0.837	0.237	0.855
15	0.786	0.289	0.795
20	0.674	0.326	0.698
22	0.602	0.455	0.602
25	0.535	0.347	0.518
30	0.426	0.309	0.427
32	0.338	0.254	0.354
35	0.225	0.186	0.246
40	0.147	0.123	0.182
45	0.053	0.003	0.065
50	0.000	0.000	0.000

Table T5: An evaluated result of column integrated momentum distribution in the far field ($r \rightarrow \infty$), total momentum distribution n(k), condensate momentum distribution n_0(k) and non condensate momentum distribution n_{nc}(k) as a function of k(π/a). Others parameters are same as in table T1.

k(π/a).	n(k)X10^{-3}	n_0(k)X10^{-3}	n_{nc}(k)X10^{-3}
-0.20	0.008	0.005	0.001
-0.15	0.025	0.018	0.003
-0.10	0.056	0.047	0.006
-0.08	0.128	0.116	0.026
-0.05	2.357	0.409	0.143
0.00	4.875	4.187	0.367
0.05	3.165	3.053	0.304
0.10	2.245	2.486	0.108
0.12	1.046	1.127	0.012
0.15	0.067	0.098	0.009
0.18	0.015	0.062	0.000
0.20	0.006	0.008	0.000
0.22	0.000	0.000	0.000

Table T6: An evaluated result of column integrated momentum distribution in the far field ($r \rightarrow \infty$), total momentum distribution n(k), condensate momentum distribution n_0(k) and non condensate momentum distribution n_{nc}(k) as a function of k(π/a). Others parameters are same as in table T3.

k(π/a).	n(k)X10^{-3}	n_0(k)X10^{-3}	n_{nc}(k)X10^{-3}
-0.20	0.000	0.000	0.000
-0.15	0.000	0.000	0.058
-0.10	0.000	0.000	0.122
-0.08	1.059	1.106	0.246
-0.05	2.546	2.649	0.348
0.00	15.246	14.986	0.685
0.05	13.248	12.242	0.504
0.08	6.387	7.059	0.365
0.10	1.546	2.127	0.217
0.15	0.058	1.059	0.178
0.18	0.015	0.062	0.102
0.20	0.009	0.054	0.046
0.22	0.000	0.000	0.005

Table T7: An evaluated result of column integrated momentum distribution in the far field ($r \to \infty$), total momentum distribution n(k), condensate momentum distribution $n_0(k)$ and non condensate momentum distribution $n_{nc}(k)$ as a function of k(π/a). Others parameters are same as in table T2.

k(π/a).	$n(k)X10^{-3}$	$n_0(k)X10^{-3}$	$n_{nc}(k)X10^{-3}$
-0.20	0.000	0.000	0.000
-0.15	0.000	0.000	0.024
-0.10	0.056	0.037	0.056
-0.08	0.092	0.076	0.106
-0.05	2.158	1.957	0.158
0.00	3.546	3.168	0.224
0.05	2.258	2.109	0.174
0.08	1.073	1.184	0.106
0.10	0.084	0.096	0.072
0.15	0.038	0.047	0.035
0.18	0.003	0.008	0.009
0.20	0.000	0.000	0.002
0.22	0.000	0.000	0.000

Table T8: **An evaluated result of column integrated momentum distribution in the far field ($r \to \infty$), total momentum distribution n(k), condensate momentum distribution $n_0(k)$ and non condensate momentum distribution $n_{nc}(k)$ as a function of k(π/a). Others parameters are same as in table T4.**

k(π/a).	$n(k)X10^{-3}$	$n_0(k)X10^{-3}$	$n_{nc}(k)X10^{-4}$
-0.20	0.000	0.000	0.058
-0.15	0.000	0.000	0.076
-0.10	0.085	0.062	0.085
-0.08	0.124	0.138	0.126
-0.05	0.586	0.657	0.248
0.00	10.258	9.857	2.056
0.05	8.456	7.242	1.253
0.08	4.586	5.086	1.158
0.10	0.156	0.146	0.076
0.15	0.058	0.067	0.065
0.18	0.006	0.008	0.009
0.20	0.000	0.000	0.002
0.22	0.000	0.000	0.000

Table T9: An evaluated result of column integrated momentum distribution for finite TOF (time of flight measurement)(τ=20ms),total momentum distribution n(k), condensate momentum distribution $n_0(k)$ and non condensate momentum distribution $n_{nc}(k)$ as a function of k(π/a). Others parameters are same as in table T1.

k(π/a).	$n(k)X10^{-3}$	$n_0(k)X10^{-3}$	$n_{nc}(k)X10^{-4}$
-0.20	0.005	0.008	0.453
-0.15	0.065	0.078	0.568
-0.10	0.092	0.105	0.674
-0.08	0.156	0.195	0.706
-0.05	0.248	0.265	0.735
0.00	2.056	1.895	0.846
0.05	1.867	1.746	0.759
0.08	0.569	0.667	0.723
0.10	0.324	0.429	0.646
0.15	0.208	0.316	0.567
0.18	0.148	0.167	0.454
0.20	0.067	0.084	0.423
0.22	0.006	0.008	0.406

Table T10: An evaluated result of column integrated momentum distribution for finite TOF (time of flight measurement)(τ=20ms),total momentum distribution n(k), condensate momentum distribution $n_0(k)$ and non condensate momentum distribution $n_{nc}(k)$ as a function of k(π/a). Others parameters are same as in table T2.

k(π/a).	$n(k)X10^{-3}$	$n_0(k)X10^{-3}$	$n_{nc}(k)X10^{-4}$
-0.20	0.000	0.000	0.467
-0.15	0.000	0.000	0.428
-0.10	0.008	0.010	0.396
-0.08	0.056	0.047	0.347
-0.05	0.124	0.119	0.316
0.00	2.864	2.538	0.673
0.05	2.547	1.987	0.148
0.08	1.674	1.743	0.098
0.10	0.846	0.737	0.248
0.15	0.532	0.508	0.336
0.18	0.308	0.298	0.454
0.20	0.194	0.175	0.592
0.22	0.065	0.038	0.327

Table T11: An evaluated result of column integrated momentum distribution for finite TOF (time of flight measurement)(τ=20ms),total momentum distribution n(k), condensate momentum distribution $n_0(k)$ and non condensate momentum distribution $n_{nc}(k)$ as a function of k(π/a). Others parameters are same as in table T3.

k(π/a).	n(k)X10^{-3}	n_0(k)X10^{-3}	n_{nc}(k)X10^{-4}
-0.20	0.000	0.000	0.422
-0.15	0.058	0.067	0.486
-0.10	0.127	0.138	0.522
-0.08	0.246	0.250	0.678
-0.05	0.387	0.392	0.724
0.00	1.584	1.606	0.635
0.05	1.039	1.032	0.606
0.08	0.946	0.907	0.675
0.10	0.638	0.612	0.642
0.15	0.349	0.322	0.615
0.18	0.176	0.166	0.462
0.20	0.095	0.087	0.317
0.22	0.006	0.004	0.279

Table T12: An evaluated result of column integrated momentum distribution for finite TOF (time of flight measurement)(τ=20ms),total momentum distribution n(k), condensate momentum distribution $n_0(k)$ and non condensate momentum distribution $n_{nc}(k)$ as a function of k(π/a). Others parameters are same as in table T4

k(π/a).	n(k)X10^{-3}	n_0(k)X10^{-3}	n_{nc}(k)X10^{-4}
-0.20	0.000	0.000	2.167
-0.15	0.048	0.067	2.108
-0.10	0.096	0.108	2.674
-0.08	0.138	0.146	4.160
-0.05	0.256	0.264	3.954
0.00	2.567	2.606	0.056
0.05	2.412	2.150	0.098
0.08	1.897	1.866	0.145
0.10	0.674	0.532	4.156
0.15	0.406	0.384	3.958
0.18	0.218	0.197	3.267
0.20	0.117	0.092	2.865
0.22	0.056	0.044	2.973

CONCLUSION:

From the above theoretical analysis and investigations, we have come across the following conclusions

(4) We have studied the effects of interactions on the components of the spatial and momentum distributions of bosonic particles in a trapped optical lattice

(5) We have evaluated condensate and non condensate spatial and momentum distributions of the Bose-Hubbard model in a trap. We have studied the above distributions at far field ($r \rightarrow \infty$) and for finite TOF. We observe that both n (K) and n^{τ}(K) are broader for large U/t.

(6) We observed that the strong interactions cause condensate to develop a structure around the central peak very much like non condensate atoms.

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