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A COULOMB POTENTIAL INTERACTING MODEL OF BOSE - EINSTEIN CONDENSATION

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ABSTRACT

In this paper, we have investigated the formation of Bose-Einstein condensation from the interaction of bosons in a modified Hubbard model which has a kinetic energy part and a Coulomb potential to control the interaction. Using the highly simplified correlated variation approach (HSCVA), we are able to obtain the ground state energy and pair correlation function (PCF) for an N x N x N = 5 x 5 x 5 lattice at positive and negative values of the interaction strength. Analysis of these results enables us to determine the repulsive and attractive regions of the model from which the conventional and non-conventional Bose-Einstien condensation can be obtained respectively.

KEYWORDS: Bosons, Bose-Einstein condensation, Perfect Bose gas, Imperfect Bose gas, Hubbard model.

INTRODUCTION

It is a common knowledge today that all particles can be divided into two big classes called fermions and bosons. The fermions have half-integer spins and consequently obey the Pauli exclusion principle which states that no two identical fermions can be in the same quantum state at the same time. The physical implication is that fermionic systems will have many energetic particles flying around even as the temperatures goes down to zero as only one particle can occupy the lowest energy. In general, fermions are governed by the Fermi-Dirac distribution (FDD).

The bosons, however, have integer spins and consequently do not obey the Pauli exclusion principle. The rules governing the behaviour of photon which is the commonest boson, were first given by Satyendra Nath Bose in 1924. Excited by this work, Einstein in the same year extended the rules to other bosons and thereby gave birth to the Bose-Einstein distribution (BED). While doing this, Einstein found that not only is it possible for two bosons to share the same quantum state at the same time, but that they actually prefer doing so. He therefore predicted that when the temperature goes down, almost all the particles in a bosonic system would congregate in the ground state even at a finite temperature. It is this physical state that is called Bose-Einstein condensation (BEC). Thus a Bose system that condensate purely due to the BED is called perfect Bose gas (PBG) (van den Berg and Lewis 1982; Pule 1983; Zegrebnov 1999; 2000; Bru and Zegrebnov 2000a; 2000b). The magnitude of the condensation of the PBG strongly depends on the shape of container and the kinetic energy of the particles (van den Berg 1983; Pule 1983).

The Einstein's prediction however was considered a mathematical artifact for sometime until Fritz London in 1938 while investigating superfluid liquid helium realized that the phase transition could be accounted for in terms of BEC. This analysis however suffered a major set back because the helium atoms in the liquid interacted quite strongly. This was why scientists had to move ahead in search of BEC in less complicated systems that would be close to the free boson gas model. Fortunately, the breakthrough came in 1995 when the first BEC was observed in rubidium atoms (Anderson et al. 1995; Cornell 1996) and this was followed by similar observations in some other cold alkali atoms such as those of lithium and sodium (Davis et al. 1995; Kirsten and Toms, 1996). Though these Bose systems manifesting condensation are gaseous, they are far from perfect because they are influenced by interactions (Davis et al 1995; Bru and Zagrebnov 2000a; 2000b). For example, Davis et al. (1995) observed that in a condensate of sodium atoms, interaction seems to predominate compared to the Kinetic energy. The implication is that real Bose systems manifesting condensation are not purely due to the BED as such they are now referred to as imperfect Bose gas (IBG). If the IBG condensation is due to repulsive interaction, it is called conventional Bose-Einstein condensation (CBEC) and when it condensate due to attractive interaction, it is called non conventional Bose-Einstein condensation (NBEC) (van den Berg et al 1984; Michoel and Verbeure 1999; Zegrebnov 1999; Bru and Zagrebnov 2000a; 2000b). Consequently, the current theoretical search is for a model of interacting bosons that will produce the two kinds of condensates (Bru and Zegrebnov 2000a; 2000b).

Since results in the literature show that the Hubbard model for electronic interactions has both repulsive and attractive regions depending on the interaction strength (Enaibe and Idiodi 2002; Akpojotor and Idiodi 2004a: 2004b), it is therefore considered a natural candidate to investigate the interacting bosons. In a preliminary report (Akpojotor and Ojobor 2006) in which we compared the two-electron variational Hubbard interactions with that modified for two-charged bosons in N = 2, N x N = 4 x 4 and N x N x N = 5 x 5 x 5 lattices, the results show only slight difference in the matrices obtained for the two kinds of particles. This slight difference did not, however, make the trend observed for the ground state energy and variational parameters of the electronic interactions to differ from those of the bosons for the N = 2 case specifically considered. This is enough motivation to compute in this present study, the pair correlation function (PCF) in order to determine the repulsive and attractive regions of the modified Hubbard bosonic interactions.

It was pointed out in the preliminary report that there are three basic steps to use the highly simplified correlated variational approach (HSCVA) to investigate the two-charged boson Hubbard interaction. The first step is to obtain the matrix representation of the interaction given by (Akpojotor and Idiodi 2004a; 2004b; Akpojotor and Ojobor 2006).

$$(H_{l_c l'} - IE)X_{l_c} = E_{\delta l_c l'} - 4\left(\frac{U}{4t}\right)_{00} + 2T_{l_c l'}, \quad (1.1)$$

where E is the ground state energy, I is a unit matrix, X are the variational parameters, Lc is the separation of the states before the Hubbard interaction, L' are the separations of the

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new states produced by using the modified Hubbard Hamiltonian to operate on a state with Lc and the T is the number of such new state for the various L^1.

The H in Eq. (1.1) is a single band Hubbard Hamiltonian modified for charged bosons and it is given by

$$H = -t\left[\sum_{<i,j>} C_i^+ C_j + H.C.\right] + U\sum_i n_i n_i \qquad (1.2)$$

where $C_i^+(C_j)$ and n_i are respectively the creation (annihilation) and number operators for bosons in the Wannier state on the ith(jth) site, H.C. is the Hermitian conjugate, U is the onsite Coulomb potential for interacting charged particles and t determine the kinetic interaction, hence the U/4t in Eq. (1.1) is the interaction strength.

The second step is to obtain the eigenvalues and eigenvectors of the matrix and the smallest of them for a particular interaction is its ground state energy while its corresponding eigenvectors are the variational parameters needed to compute the PCF in the third step.

The plan of this present study is as follows. Since we had shown in the preliminary report how to use the HSCVA to obtain the matrix representations of the modified Hubbard Hamiltonian two boson interactions in N = 2, N x N = 4 x 4 and N x N x N = 5 x 5 x 5 as well as how to obtain numerically the ground state energies and variational parameters for N = 2, we hope solving the matrices numerically for the remaining lattices is straightforward. So in sec. II, we will derive a general expression for the PCF in terms of the variational parameters and the total number of bosonic states in a given separation. This expression will then be applied only to N x N x N = 5 x 5 x 5. Our choice of application emanates from observations made in previous studies (Enaibe and Idiodi 2002; Akpojotor and Idiodi 2004a; 2004b) that the trend in any dimension studied are usually consistent in the other dimensions. Further, the three dimensional (3D) lattices will be able to accommodate the random motion in all spatial directions of the Bose gas more than the lower dimensions. The results from the application will be presented and discussed in sec III and this will be followed by a conclusion.

PAIR CORRELATION FUNCTION (PCF)

In general, the pair correlation function is defined as the conditional probability of finding a particle at site j when there is another particle fixed at site i (Petukhov et al. 1992). It is expressed mathematically as

$$P_{(i,j)} = \frac{\langle \psi / n_{i\sigma} n_{j\sigma} / \psi \rangle}{\langle \psi / \psi \rangle} \qquad (2.1)$$

where n_i (= $C_i^+ C_i$) retains its definition, σ which is the spin projection is neglected for the bosons and the ket, $/\psi>$, in the Hilbert space is the wavefunction of the physical system under consideration and it is defined as (Akpojotor and Idiodi 2004a; 2004b; Akpojotor and Ojobor 2006)

$$/\psi> = \sum_{L_c=0}^{S-1} X_{L_c} /\psi_{L_c}> \qquad (2.2)$$

while its bra as

$$<\psi / = \sum_{L_c=0}^{S-1} X_{L_c} <\psi_{L_c} / . \qquad (2.3)$$

In Eqs (2.2) and (2.3), the X and Lc retain their earlier definitions while S is the total number of possible separations in a given lattice (Akpojotor et al. 2002; 2006). Taking into account the two equations, it can be shown by mere expansion that

$$<\psi/\psi> = \sum_{L_c=0}^{S-1} n_{L_c} X_{L_c}^2 \qquad (2.4)$$

where the n_{L_c} denotes the total number of bosonic states having separation Lc. See Akpojotor et al. (2006) on how to determine the n_{L_c}.

Similarly it can be shown that by expanding the number operators for both onsite separations and the intersite separations and using them to operate on the ket and then introducing the bra, the numerator in Eq (2.1) becomes for onsite separations,

$$\langle \psi / n_i n_i / \psi \rangle = X_0^2 \qquad (2.5)$$

and for intersite separations,

$$\langle \psi / n_i n_j / \psi \rangle = 2X_{L_c}^2 . \qquad (2.6)$$

Finally, taking into account Eqs (2.4) - (2.6) in Eq. (2.1), the PCF can now be expressed in terms of the variational parameters and the total number of state in a given separation as

$$P_{L_c=0} = \frac{X_0^2}{\sum_{L_c=0}^{S-1} n_{L_c} X_{L_c}^2} \qquad (2.7)$$

for onsite interactions and for intersite interactions

$$P_{L_c} = \frac{2X_{L_c}^2}{\sum_{L_c=0}^{S-1} n_{L_c} X_{L_c}^2} \qquad (2.8)$$

Eqs. (2.7) and (2.8) are applied to N x N x N = 5 x 5 x 5 using the variational parameters obtained from the solution of its matrix representation by considering the following arbitrary values for the interaction strength: U/4t = 10, 5, 2, 1.5, 1, 0.5, 0, -0.5, -1, -1.5, -2, -5, -10. The results are shown in Table 1.

PRESENTATION AND DISCUSSION OF RESULTS

In Table 1 which shows the interaction strength, the ground state energy and pair correlation function for N x N x N = 5 x 5 x 5, it is observed that the ground state energy of the two interacting charged bosons are negative, non-degenerate and decreases as U/4t is decreased. This is the same observation made for both the electronic and bosonic interactions in N = 2 considered in the preliminary report.

Table 1: The ground state energy and pair correlation function (PCF) at positive and negative values of the interaction strength for the two-charged boson modified Hubbard interactions on N x N x N = 5 x 5 x 5.

Interaction Strength U/4t	Ground State Energy E	Pair Correlation Function (PCF)									
		P_0	P_1	P_2	P_3	P_4	P_5	P_6	P_7	P_8	P_9
10.0	-11.8374	0.0000288	0.000393	0.000624	0.000709	0.000684	0.000743	0.000776	0.000793	0.000811	0.000834
5.0	-11.8449	0.0000387	0.000411	0.000631	0.000713	0.000688	0.000744	0.000776	0.000792	0.000810	0.000831
2.0	-11.8580	0.0000667	0.000442	0.000644	0.000719	0.000697	0.000748	0.000777	0.000792	0.000808	0.000827
1.5	-11.8622	0.0000759	0.000452	0.000648	0.000721	0.000699	0.000749	0.000777	0.000792	0.000807	0.000826
1.0	-11.8677	0.0000879	0.000465	0.000652	0.000724	0.000703	0.000751	0.000778	0.000792	0.000806	0.000825
0.5	-11.8753	0.0001040	0.000483	0.000661	0.000727	0.000708	0.000753	0.000778	0.000791	0.000805	0.000822
0.0	-11.8862	0.0001290	0.000510	0.000673	0.000733	0.000715	0.000756	0.000780	0.000791	0.000804	0.000819
-0.5	-11.9033	0.0001670	0.000552	0.000691	0.000742	0.000727	0.000762	0.000782	0.000792	0.000803	0.000816
-1.0	-11.9337	0.0002370	0.000628	0.000725	0.000760	0.000750	0.000774	0.000787	0.000794	0.000801	0.000810
-1.5	-12.0000	0.0004020	0.000803	0.000803	0.000803	0.000803	0.000803	0.000803	0.000803	0.000803	0.000803
-2.0	-12.2034	0.0010040	0.001406	0.001068	0.000946	0.000984	0.000904	0.000860	0.000839	0.000817	0.000790
-5.0	-20.9370	0.0074900	0.002340	0.000493	0.000153	0.000287	0.000092	0.000037	0.000024	0.000012	0.000004
-10.0	-40.3711	0.0079220	0.000979	0.000100	0.000014	0.000052	0.000007	0.000001	0.000001	0.000000	0.000000

Further, it is observed that the onsite PCF increases from P_0 = 0.0000228 as the interaction strength is decreased from U/4t = 10 to P_0 = 0.007922 at U/4t = -10 while the largest intersite separation decreases from $P_{S-1} = P_9$ = 0.000834 at U/4t = 10 to P_9 = 0 at U/4t = -10. The implication is that when the repulsive interaction strength is large, the probability of finding the bosons as far apart as possible is high while that of finding the bosons on the same site is very low. The reverse is the case when the attractive interaction dominates as the bosons now prefer to be on the same site while the probability of finding the particles as far apart as possible tends to zero. It is pertinent to point out here that even when the bosons prefer to stay as far part as possible in the repulsive interaction, they don't fly out of the ground state. In other words, the gregarious behaviour of bosons is not distorted by the repulsive interaction.

Another interesting observation from our table is that the system was still repulsive when the interaction strength is switched off, that is, U/4t = 0. This is why the PCF decreases from the largest separation $P_{S-1} = P_9$ = 0.000819 to that of the smallest separation P_0 = 0.000129. This is contrary to our expectation that the transition from the repulsive region to the attractive region should be when the interaction strength is switched off, because the bosonic system will now be left with only the kinetic part of the model Hamiltonian in Eq. (1.2) and this part should naturally be a perfect Bose gas. This PBG should have the same energy for lattices of the same dimensions and the bosons should have equal preference to stay on any site so that the PCF will be the same for all separations. It is observed from the table, however, that the bosons prefer to stay together on any site when U/4t = -1.5 and the ground state energy is E = -12.0000. Further investigation of other lattices in all three dimensions, shows that at precisely U/4t = - 0.5, U/4t = – 1. 0 and U/4t = –1.5, the ground state energies are respectively E = -4.0000 for 1D systems, E = -8.0000 for 2D systems and E = -12.0000 for 3D systems and that the PCF are the same for all the intersite separations. These values of the interaction strength are therefore the transition points from the repulsive region to the attractive region in the various dimensions. This is a very interesting observation as it implies that BEC cannot be realised purely from the kinetic energy of the particles. In other words, it is not possible to have BEC from a PBG driven only by the kinetic energy of the bosons. Thus we have shown theoretically why the experimentally observed Bose systems manifesting BEC are influenced by interactions.

CONCLUSION

We have set out in this study to determine the repulsive and attractive regions to determine the conventional BEC and non conventional BEC in the two-charged boson modified Hubbard variation interactions. These regions have been duly observed in the model and consequently we now have a rough estimate of the parameter space for studying the two kinds of condensation from an imperfect Bose gas. It is recommended therefore that for the application of the model to actual Bose systems, more detailed studies have to be done to determine the parameter space for each particular case. Another interesting observation is that the perfect Bose gas cannot

manifest condensation purely from the kinetic energy of the particles. This is very crucial as our theoretical model have given insight into why real systems manifesting condensation have always been influenced by interactions. Perhaps this aspect of the study can be investigated further by enhancing only the kinetic part of our model to see if it will manifest condensation without any form of interactions.

Conclusively, it is pertinent to emphasize here as we have done previously (Akpojotor and Ojobor 2006) that the possibility of obtaining both superconductivity and Bose-Einstein condensation from the same model is quite enticing. This promise of unity of two of the most important low temperature phenomena is a worthy challenge for both theorists and experimentalists.

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