GLOBAL JOURNAL OF PURE AND APPLIED SCIENCES, VOL. 12 NO 1, JANUARY, 2006: 119-123
COPYRIGHT (C) BACHUDO SCIENCE CO. LTD. PRINTED IN NIGERIA. ISSN 1118-0579

COMPARISON OF A TWO ELECTRON WITH A TWO CHARGED BOSON VARIATIONAL HUBBARD INTERACTIONS

G. E. AKPOJOTOR and S. A. OJOBOR

(Received 17 June, 2004; Revision Accepted 10 November, 2004)

ABSTRACT

There is growing belief that both the conventional Bose Einstein condensation (CBEC) and non-conventional Bose Einstein condensation (NBEC) can be obtained from repulsive and attractive interactions of bosons respectively. However, there is still no generally accepted model to obtain both condensates. Since results in the literature show that the Hubbard model two electron interactions has both repulsive and attractive regions depending on the interaction strength, we are considering its extension to charged bosons to investigate the possibility of obtaining the condensates from it. As a preliminary investigation, we have compared in this present study, the two electron variational Hubbard Hamiltonian with that modified for 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 differences between the cases of the electrons and bosons. The implication that there is possibility of obtaining both condensates from the Hubbard model is then discussed in relation to superconductivity.

KEYWORDS: Bose Einstein condensation, superconductivity, Hubbard model, electrons, bosons.

INTRODUCTION

Superconductivity (SC) and Bose Einstein condensation (BEC) are two very important phenomena in low temperature physics. The former is believed to occur in superconducting materials when there is an appropriate interaction mechanism of the electrons which are fermions so that there is an energy gap between the excited states and the ground state (Akpojotor 1999). The latter occurs when there is collapse of an aggregate of bosons to a collective ground state in which they all have the same minimal ground state momentum (Liboff 1992). Recently, it has been adduced (Bru and Zagrebnov 2000) that BEC can be induced by interaction of bosons. As a matter of increasing belief, the two kinds of condensates, the conventional Bose-Einstein condensation (CBEC) and the non-conventional Bose-Einstein condensation (NBEC) can be obtained from repulsive and attractive interactions of bosons respectively (Van den Berg, Lewis and deSmedt 1984: Zagrebnov 1999: Bru and Zagrebnov 2000a: 2000b). It is very tempting, therefore, to study the interaction of bosons using a modified Hubbard Hamiltonian since results in the literature from similar studies for the interaction of electrons, show that there are both repulsive and attractive regions in the model as one varies the size of the interaction strength (Enaibe and Idiodi 2002; Enaibe 2003; Akpojotor and Idiodi, 2004). Before embarking on such a study, it is necessary to make a preliminary comparison of the model for the interactions of the two classes of particles. This is the study we have undertaken here.

The mathematical approach for this study is the simplified formulation of the variational techniques developed recently (Akpojotor and Idiodi, 2004). This approximation technique was first developed for one and two dimensions by Chen and Mei (1989) and recently extended to three dimension by Enaibe (2003). The approach is very effective in calculating the ground state energy and wavefunction of time independent Hamiltonians (Bransden and Joachain 1989). Usually, to use the approach, there are three basic steps. The first one is to obtain the matrix representation of the Hamiltonian of the system being studied. The second is to solve this matrix to obtain its eigenvalues and eigenvectors. The smallest eigenvalue is the ground state energy and its corresponding eigenvectors are used in the third step to compute the pair correlation functions to determine the repulsive and attractive regions of the model. We will undertake the first step and then make a little incursion into the second step in this study.

The plan of this study is the following. In the next section (sec.II), we will formulate the variational technique to obtain the matrix representations of the Hubbard Hamiltonian two electron and two boson interactions in N = 2, N x N = 4 x 4 and N x N x N = 5 x 5 x 5 lattices. The results will be presented in sec. III where we will also obtain the energy spectra and wavefunctions of both Hamiltonians for N = 2. This will be followed by a conclusion.

FORMULATION OF THE VARIATIONAL ENERGY

The variational ground state energy is given by (Chen and Mei, 1989)

$$E_g = \frac{\langle \psi / H / \psi \rangle}{\langle \psi / \psi \rangle}, \tag{2.1}$$

where the H is the Hubbard Hamiltonian to be defined later for electrons and bosons while the ket in the Hilbert space is the trial wavefunction defined as

$$/\psi > \; = \; \sum_{L=0}^{S-1} X_L / \psi_L > . \tag{2.2}$$

In Eq. (2.2), the X is the variational parameter, the L is the lattice separation between the two particles and the S denotes the total number of such separations possible in a given lattice. A single lattice separation is denoted by a and all other separations are written in terms of a. Owing to the convention introduced in Akpojotor et al. (2002; 2005), L takes values from

$$L_c = 0,1,2 \ldots S-1. \tag{2.3}$$

The bra in Eq. (2.1) is that of the ket in Eq. (2.2), that is,

G. E. AKPOJOTOR, Physics Department, Delta State Univeristy, Abraka, Nigeria
S. A. OJOBOR, Mathematics Department, Delta State Univeristy, Abraka, Nigeria

$$<\psi| = \sum_{L_c=0}^{N-1} X_{L_c} <\psi_{L_c}| \qquad (2.4)$$

We have shown that without going through the often tedious procedure of the Chen and Mei (1989) approach, the matrix representation can directly be expressed as (Akpojotor and Idiodi 2004),

$$(H_{L_c L^1} - IE)X_{L_c} = E_{\delta L_c L^1} - 4\left(\frac{U}{4t}\right)_{00} + 2T_{L_c L^1} \qquad (2.5)$$

where the $E_g/t = E$ is the total energy, the U/4t is the interaction strength between the two particles, the L^1 are the separations of the new states produced by using either the two electron or two boson Hubbard model to activate a state with separation L_C and the T is the number of such new states for the various L^1.

The Two Electron Interaction

The single band Hubbard model is given by (Chen and Mei 1989)

$$H = -t\left[\sum_{<i,j>,\sigma} C_{i\sigma}^{+} C_{j\sigma} + H.C.\right] + U\sum_i n_{i\uparrow} n_{i\downarrow} \qquad (2.6)$$

where $C_{i\sigma}^{+}(C_{i\sigma})$ and $n_{i\sigma}$ are respectively the creation (annihilation) and number operators for an electron in the Wannier state on the ith (jth) lattice site with spin projection σ, H.C is the Hermitian conjugate, U is the onsite Coulomb interaction and t restrict the hopping of the electron to nearest- neighbour site.

To obtain L^1 and T, we need only the particle creation and annihilation operators of the Hubbard Hamiltonian given by

$$H_p = \left[\sum_{<i,j>,\sigma} C_{i\uparrow}^{+} C_{j\uparrow} + C_{j\uparrow}^{+} C_{i\uparrow} + C_{i\downarrow}^{+} C_{j\downarrow} + C_{j\downarrow}^{+} C_{i\downarrow}\right] \qquad (2.7)$$

to activate a selected state in L_C (Akpojotor and Idiodi 2004). This was done for N = 2, N x N = 4 x 4 and N x N x N =5 x 5 x 5. For N=2, the two new states obtained by activating a state in L_c=0 belong to L^1 =1 hence T=2 while the two new states for L_c=1 belong to L^1 = 0 hence T = 2.

The L^1 and T obtained above are introduced into Eq. (2.5) to obtain the matrix representation of the two electron Hamiltonian on an N = 2 lattice as shown in Eq. (2.10).

The Two Charged Boson Interaction

To modify the Hubbard Hamiltonian given by Eq. (2.6) to be valid for charged bosons, all that is needed to be done is to exclude the spins and this will relax the Pauli exclusion principle which holds that two fermions with the same spins cannot occupy the same quantum state. Consequently, the Hubbard Hamiltonian for the bosons is

$$H = -t\left[\sum_{<i,j>} C_i^{+} C_j + H.C.\right] + U\sum_i n_i n_i \qquad (2.8)$$

and Eq. (2.7) becomes

$$H_p = \left[\sum_{<i,j>} C_i^{+} C_j + C_j^{+} C_i\right] \qquad (2.9)$$

As in the case of electrons, the above equation was used to activate selected states in the various separations in N = 2, N x N = 4 x 4 and N x N x N =5 x 5 x 5. We observe that for N = 2, only one new state was obtained by activating a state in L_c=0 so that L^1 =1 and T=1 while the two new states for L_c=1 belong to L^1 = 0 hence T = 2.

The L^1 and T obtained above are introduced into Eq. (2.5) to obtain the matrix representation of the two boson Hamiltonian on an N = 2 lattice as shown in Eq. (2.13).

PRESENTATION OF RESULTS

The L^1 and T of N x N= 4 x 4 and N x N x N= 5 x 5 x 5 are obtained both for the two electron and two boson cases using the same procedure shown for N = 2 in the preceding section. They are then introduced into Eq. (2.5) to obtain the matrix representations of the Hamiltonians for the respective lattices considered as shown in Eqs. (2.10 – 2.15).

$$\begin{bmatrix} E-4\left(\frac{U}{4t}\right) & 2 \\ 2 & E \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \end{bmatrix} = 0 \qquad (2.10)$$

$$\begin{bmatrix} E-4\left(\frac{U}{4t}\right) & 8 & 0 & 0 & 0 & 0 \\ 2 & E & 4 & 2 & 0 & 0 \\ 0 & 4 & E & 0 & 4 & 0 \\ 0 & 4 & 0 & E & 4 & 0 \\ 0 & 0 & 4 & 2 & E & 2 \\ 0 & 0 & 0 & 0 & 8 & E \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \end{bmatrix} = 0 \qquad (2.11)$$

$$\begin{bmatrix} E-4\left(\frac{U}{4t}\right) & 12 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 2 & E & 8 & 0 & 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 4 & E & 4 & 0 & 4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 6 & E & 0 & 0 & 6 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & E+2 & 8 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 2 & E+2 & 4 & 2 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 4 & E+2 & 0 & 4 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4 & 0 & E+4 & 4 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 4 & 2 & E+4 & 2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 6 & E+6 \end{bmatrix} \begin{bmatrix} X_0 \\ X_1 \\ X_2 \\ X_3 \\ X_4 \\ X_5 \\ X_6 \\ X_7 \\ X_8 \\ X_9 \end{bmatrix} = 0 \qquad (2.12)$$

$$\begin{bmatrix} E-4\left(\frac{U}{4t}\right) & 1 \\ 2 & E \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \end{bmatrix} = 0 \qquad (2.13)$$

$$\begin{bmatrix} E-4\left(\frac{U}{4t}\right) & 4 & 0 & 0 & 0 & 0 \\ 2 & E & 4 & 2 & 0 & 0 \\ 0 & 4 & E & 0 & 4 & 0 \\ 0 & 4 & 0 & E & 4 & 0 \\ 0 & 0 & 4 & 2 & E & 2 \\ 0 & 0 & 0 & 0 & 8 & E \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \end{bmatrix} = 0 \qquad (2.14)$$

$$\begin{bmatrix} E-4\left(\frac{U}{4t}\right) & 6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 2 & E & 8 & 0 & 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 4 & E & 4 & 0 & 4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 6 & E & 0 & 0 & 6 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & E+2 & 8 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 2 & E+2 & 4 & 2 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 4 & E+2 & 0 & 4 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4 & 0 & E+4 & 4 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 4 & 2 & E+4 & 2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 6 & E+6 \end{bmatrix} \begin{bmatrix} X_0 \\ X_1 \\ X_2 \\ X_3 \\ X_4 \\ X_5 \\ X_6 \\ X_7 \\ X_8 \\ X_9 \end{bmatrix} = 0 \qquad (2.15)$$

From Eqs. (2.10 – 2.15), it is easy to observe that the matrices of the two electron Hubbard Hamiltonian and their equivalents for the two boson modified Hubbard Hamiltonian are the same except for the element H_{01} where in all dimensions, that of electron interaction is twice that of the boson interaction.

To have an insight into how this little difference in the matrix element H_{01} could affect the energy spectra and wavefuntion, we will determine the energy spectra and variiational parameters of both Hamiltonians for the case of N = 2 by using Eqs (2.10) and (2.13).

The Two Electron Interaction on N = 2

Observe that Eq. (2.10) is the matrix form of the eigenvalue problem (Harper 1989). Therefore we can obtain the eigenvalue, E by demanding that to obtain a non-trivial solution, its determinant must be zero i.e

$$\left| H_{l,l'} - IE \right| = 0 \quad (3.1)$$

This will yield a quadratic equation;

$$E^2 - 4\left(\frac{U}{4t}\right)E - 4 = 0 \quad (3.2)$$

which can be resolved by using the simple Almighty formular as

$$E = 2\left\{\left(\frac{U}{4t}\right) \pm \sqrt{\left(\frac{U}{4t}\right)^2 + 1}\right\} \quad (3.3)$$

The smallest root which is the smallest eigenvalue is the ground state energy,

$$E_0 = 2\left\{\left(\frac{U}{4t}\right) - \sqrt{\left(\frac{U}{4t}\right)^2 + 1}\right\} \quad (3.4)$$

The Two Boson Interaction on N = 2

If we follow the same procedure to resolve the matrix form of the two boson modified Hubbard Hamiltonian in Eq. (2.13), we will obtain the ground state energy as

$$E_0 = 2\left[\left(\frac{U}{4t}\right) - \sqrt{\left(\frac{U}{4t}\right)^2 + \frac{1}{2}}\right] \quad (3.5)$$

Several arbitrary values are chosen for the interaction strength such as U/4t=10, 5, 0, -5 and −10 and then substituted into Eqs. (3.4) and (3.5) to compute for the ground state energies of the different Hamiltonians. Thereafter, the corresponding eigenvectors which are the variational parameters are obtained. The results are shown in Table1.

Table1: Comparison of the total energies and variational parameters for two electron and two boson variational Hubbard interactions on an N = 2 lattice.

Interaction stenght U/4t	Electrons			Bosons		
	Total energy $E = E_g/t$	Variational parameters		Total energy $E = E_g/t$	Variational parameters	
		X_0	X_1		X_0	X_1
10	-0.0998	0.0498	0.9988	-0.0499	0.0250	0.9997
5	-0.1980	0.0985	0.9951	-0.0995	0.0497	0.9988
0	-2.0000	0.7071	0.7071	-1.4142	0.5774	0.8165
-5	-20.1980	0.9951	0.0985	-20.0995	0.9951	0.0990
-10	-40.0998	0.9988	0.0498	-40.0499	0.9988	0.0499

In Table 1, we observe that the total energy of the two interacting electrons is negative, non-degenerate and decreases as U/4t is decreased. This observation is consistent in the case of the two interacting bosons. The implication is that for both types of interactions, the interaction between the particles is enhanced as the interaction strength is decreased.

Further, we observe that for the variational parameters of the two interacting electrons, the X_0 increases as U/4t is decreased while the X_1 decreases as the U/4t is decreased. This is also the trend for the two interacting bosons. The implication is that for both types of interactions, the interacting particles prefer to stay apart on different sites when the interaction strength is increased above zero while they prefer to stay together on the same site when it is decreased below zero.

CONCLUSION

The results obtained in this study are so encouraging that it will not be naive not to expect any major abnormality when we shall compute the pair correlation function (PCF) to determine the repulsive and attractive regions of the modified Hubbard Hamiltonian for bosons. We excitedly foresee an interesting scenario where a single model, the Hubbard model, perhaps with appropriate modifications, will be used to obtain and probably account for the physics of the two most important phenomena in low temperature physics, superconductivity and Bose Einstein condensation.

ACKNOWLEDGMENT

One of us, GEA, acknowledges Prof. Valentine V Zagrebnov for sending him the preprints of his published works on Bose Einstein condensation.

REFERENCES

Akpojotor, G. E.,1999. Review of the Hubbard-like and t-J like models of superconductivity. M.Sc Thesis, University of Benin, Benin City, Nigeria.1pp.

Akpojotor, G. E., Enaibe E.A. and Ojobor S.A., 2005. A method to obtain the bosonic states in any two boson lattice system. To be publish in Global J. Pure and Applied Sc.

Akpojotor, G. E. and Idiodi, J.O., 2004. A highly simplified variational formulation of the two electron t-U and t-t^1-U models. Zuma J. Pure and Applied Sc. 6(1): 24 – 128.

Akpojotor, G. E, Idiodi, J. O., Enaibe, E. A. and Enukpere, E., 2002. A method to determine the states in two electron lattice system. Nig. J. Phys. 14 (2):117-121.

Bransdon, B. H. and Joachain, C. J., 1989. Introduction to Quantum Mechanics, John Wiley and sons Inc Nig. 379pp.

Bru, J – B and Zagrebnov, V.A., 2000a. A model with coexistence of two kinds of Bose condensation. J. Phys a: Math Gen 33: pp – 464.

Bru, J – B and Zagrebnou V.A., 2000b. On condensation in the Bogoliubou weakly imperfect Bose Gas. J. Stat. Phys. 99: 297 – 1338.

Chen, L. and Mei, C., 1989. Exact calculation of the two electron interaction in the ground states of the Hubbard model. Phys. Rev. B39: 9006-9011.

Enaibe, E. A., 2003. A variational approach to the study of highly correlated electron systems Ph. D Thesis, University of Benin, Benin City., Nigeria. Chapter four.

Enaibe, E. A and Idiodi, J.O 2002. A variational approach to the study of strongly correlated electron systems. J. Nig. Ass. Math. Phys.6: 63-73.

Harper, C., 1989. Introduction to Mathematical Physics. Prentice-Hall of India Private Limited, New Delhi, 58pp.

Libboff, R. L., 1992. Introductory Quantum Mechanics (2nd Ed) Adision – Weslev Publishing Co. Inc 612pp.

Van den Berg, M., Lewis J.T. and Ph de Smedt., 1984. Condensation in the imperfect boson gas. J. Stat. Phys. 37: 697 – 716.

Zagrebnov, V. A., 1999. The Bogoliubov Weakly imperfect Bose gas. J. Physical studies 3: 239 – 251.