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A METHOD TO OBTAIN THE BOSONIC STATES IN ANY TWO BOSON LATTICE SYSTEM

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ABSTRACT

The total number of states of any system is produced by all the possible interactions of the particles in that system. It follows therefore that there is need to obtain the states of the system before a model can be applied to it. Recently we developed a simple method to obtain the electronic states in the two electron lattice systems in all the three dimensions. This method encompasses rules formulated from a detailed study of each dimension. In the current study, the method will be extended to bosons which do not obey the Pauli exclusion principle like the electrons so that their interactions are different from those of the latter. The need for the extension of the method to bosons is also discussed in the work.

KEYWORDS: Lattices, bosons, fermions, interactions, bosonic states.

INTRODUCTION

The wave function of a physical system not only determines the properties of the system at the instant it is given but can also be used to simulate properties of the system at other instants. This is because the wave function consists of all the states of the particles which are all their possible interactions. Apart from the separation between the particles, another quantity that determines the interactions are the spins of the particles (Chen and Mei 1989; Petuhkov et al.1992: Eder et al.1996). Bosons have zero or integral spins unlike fermions which have half integral spins. Bosons therefore have symmetric wave functions because the states within them are symmetric. Fermions, on the contrary, have antisymmetric wave functions because the states within them are antisymmetric. These wave functions are appropriate to systems containing identical particles (Libboff 1992). There is a fundamental distinction between the classical and quantum descriptions of such systems. In the classical description, identical particles are distinguishable as such one may conceptually label such particles and follow their respective motions. At the quantum level of description, identical particles are indistinguishable and this is why their spins become very important in determining their interactions.

Consider for example two identical particles (fermions or bosons) on a three dimensional (3D) lattice. If the first one is on site (x,y,z) and the second on site (x^1,y^1, z^1) then the state will be

$$/ xyz\sigma, x^1y^1z^1\bar{\sigma} > \qquad (1.1)$$

where x, y, z, x^1 , y^1 and z^1 represent the positions of the particles in spatial dimensions and $\sigma(\bar{\sigma}) = (\uparrow\downarrow),(\downarrow\uparrow),(\uparrow\uparrow),(\downarrow\downarrow),(00)$ (i.e. spins)

It is easily observed that the fermionic states will be antisymmetric

$$/ xyz\sigma, x^1y^1z^1\bar{\sigma} >= -/ x^1y^1z^1\bar{\sigma}, xyz\sigma >, \qquad (1.2)$$

while the bosonic states will be symmetric

$$/ xyz\sigma, x^1y^1z^1\bar{\sigma} >=/ x^1y^1z^1\bar{\sigma}, xyz\sigma >. \qquad (1.3)$$

Though there is no experimental evidence to the best of our knowledge that distinguish between two states obtained by exchanged of two identical particles, it is obvious from Eqs. (1.2) and (1.3) that the behaviour of fermonic states are different from those of bosons. This is due to the Pauli exclusiom principle which holds that two fermions cannot exist in the same quantum state. Recently we developed a method to obtain the states of a two electron interactions on any lattice in all the three dimensions (Akpojotor et al. 2002 which is hereafter referred to as Pilot paper). That study has enabled us to developed a highly simplified formulation of the correlated variational approach (CVA) for the two electron Hubbard interactions on any lattice size in all three dimensions (Akpojotor and Idiodi 2004). The formulation can be extended to bosonic system. The need for this extension emanates from the growing opinion that both the conventional Bose Einstein condensation (CBEC) and the non-conventional Bose Einstein condensation (NBEC) can be obtained by an appropriate repulsive and attractive interactions of bosons respectively (Van den Berg, Lewis and deSmedt 1984: Zagrebnov 1999: Bru and Zagrebnov 2000a: 2000b).

Consequently, there is need to first extend the method of obtaining the two electron states to a two interacting charged bosons. This is the goal of our study here. The plan of the study is as follows. We will introduce some of the parameters needed to adopt the rules to determine the various separations in sec II. Then the rules to obtain the total number of states in the various separations will be set up in sec. III. In that sec. also, we will also compare the method with that of the two electron problem. This will be followed by a conclusion.

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RULES TO SET UP THE VARIOUS SEPARATIONS

To enhance our understanding of the study, we would like to study the two bosons, four sites (N=4) problem which is a one dimensional (1D) system before simulating for larger lattices and higher dimensions. For the bosonic states of a ID lattice, Eq (1.1) has to be rewritten only for the x direction as

$$/x,x^1> . \tag{2.1}$$

Thus the separation, L, between the two particles will be

$$L = \left|x - x^1\right| a \tag{2.2}$$

Where a is the usual lattice separation between a particle and its nearest neighbour (kittel 1996).

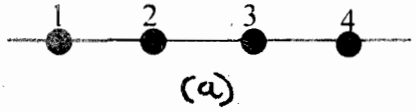
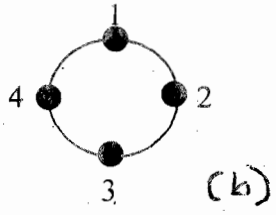


Fig.2.1 The 1D lattice with four sites (N=4): (a) without periodic boundary conditions so that there are edge effects to the left side of site 1 and to the right side of site 4, and (b) with periodic boundary conditions so that there is no edge effect on any site thereby making the lattice to be continuous.



Observe that in Fig 2.1b, the two bosons can both be on site 1,2,3 or 4 giving us onsite bosonic states with separation that is zero i.e L = 0. Consequently, the onsite states will be

$$/i,i>=/1,1>,/2,2>,/3,3>,/4,4> . \tag{2.3}$$

Also, in Fig 2.1b, the two particles could also have separation L = a, implying that if one is in a given site i, the other will be in the nearest neighbouring site, j say, thereby producing intersite bosonic states,

$$/i,j>=/1,2>,/2,3>,/3,4>,/1,4> . \tag{2.3}$$

Furthermore, the two particles could be separated by L = 2a, implying that if one boson is in site i, the other will be in the next nearest neighbour site, j say, consequently, the intersite bosonic states will be

$$/i,j>=/1,3>,/2,4> . \tag{2.3}^{**}$$

Observe that there is a total number, n, of ten states (i.e. n = 10). If we follow the same procedure of determining the states in other lattices in all the three dimensions, then it can be shown that the total number of states of any two boson lattices with periodic boundary conditions will be

$$n = {}^{K}C_2 + K = \tfrac{1}{2}(K^2 + K) \tag{2.4}$$

where K = N for 1D lattices,

$$K = N^2 \text{ for 2D lattices,} \tag{2.5}$$

and $K = N^3$ for 3D lattices,

which is different from that of the problem of two electrons in which the total number of electronic states is (Pilot paper)

$$n = \tfrac{1}{2}({}^{2K}C_2 + K) = K^2 \tag{2.6}$$

where K is also as in Eq. (2.5).

The variation in total number of states constitutes the major difference between the fermonic and bosonic systems of the same lattice size. For it can be shown from lattice diagrams of bosonic particles in all three dimensions as done for electrons in the Pilot paper that the total number of possible separations, S in 1D lattices is

$$S = \frac{N+2}{2} \text{ (for even N sites),} \tag{2.7}$$

$$S = \frac{N+1}{2} \text{ (for odd N sites),} \tag{2.8}$$

while for 2 D lattices, it is

$$S = \frac{(N+4)(N+2)}{8} \quad \text{(for even N x N sites),} \tag{2.9}$$

$$S = \frac{(N+3)(N+1)}{8} \quad \text{(for odd N x N sites),} \tag{2.10}$$

and for 3 D lattices it is

$$S = \frac{(N+6)(N+4)(N+2)}{48} \quad \text{(for even N x N x N sites),} \tag{2.11}$$

$$S = \frac{(N+5)(N+3)(N+1)}{48} \quad \text{(for odd N x N x N sites).} \tag{2.12}$$

The implication is that we can adopt for the present study the rules to set up the various separations formulated for the two electrons. Before stating these rules, we will introduce the quantities used.

It has been stated above that a separation will be denoted by L. The longest linear separation will be denoted by L_L. It usually produce the longest separation for the ID lattices while for the 2D and 3D lattices, it produces the longest diagonal lengths denoted by L_{LD} which are the longest separations for those dimensions. Every other diagonal length produced from L_L is donated by L_D while those produced by linear lengths, L_l smaller than L_L are denoted by L_d with the longest of them denoted by L_{ld}. The total number of diagonal separation depends on the linear length. It is denoted by N_d for L_l and N_D for L_L.

Using the above notations, the rules for setting the various separations are as follows

I The longest linear separation L_L for all dimensions is

$$L_L = \frac{N}{2}a \text{ for even lattices and } L_L = \frac{N-1}{2}a \text{ for odd lattices.}$$

II. The number of possible 2D diagonal lattice separations, from any linear separation is

$$N_d^{2D} = \frac{L_l}{a} \text{ and } N_D^{2D} = \frac{L_L}{a},$$

while for the 3D, it is

$$N_d^{3D} = \sum_{L_l=a}^{L_l} \frac{L_l}{a} \text{ and } N_D^{3D} = \sum_{L_l=a}^{L_l} \frac{L_L}{a}.$$

III. The various diagonal lattice separations are given by

$$L_d = L_D = \sqrt{(|x-x^1|a)^2 + (|y-y^1|a)^2 + (|z-z^1|a)^2},$$

with the longest of them as

$$L_{ld} = \sqrt{L_l^2 + L_l^2 + L_l^2} \text{ and } L_{LD} = \sqrt{L_L^2 + L_L^2 + L_L^2},$$

where x, y, z, x^1, y^1 and z^1 retain their earlier definitions as the spatial positions so that the distances between the two bosons in the respective directions will determine the separations between the two bosons in the three directions. The spatial positions take values from 1,2,3,...,L_l for L_d and 1,2,3,...,L_L for L_D.

The arrangement of separations should be by a sequential increment of the lengths of the separations, that is, if the first boson is placed on a selected site, say site (iii), then the other boson will be on the same site(iii) for onsite interaction and for intersite interactions, on

sites $[(i+1)ii], [(i+1)(i+1)i], (i+1)(i+1)(i+1)], [(i+2)ii], ..., [(i+\frac{L_L}{a})(i+\frac{L_L}{a})(i+\frac{L_L}{a})].$

To enhance the neatness of the work, we adopt a convention that the various separations shall be labelled from L_C = 0,1,2,..., S– 1, where S is as defined in Eqs. (2.7) – (2.12).

RULES TO DETERMINE THE TOTAL NUMBER OF STATES IN THE VARIOUS SEPARATIONS.

It has been stated in the preceding sec. that the variation in the total number of states constitute the major difference between fermonic and bosonic systems. This variation occurs as a result of the variation in the number of states in the equivalent separations of the respective lattice sizes. Consequently the rules to obtain the total number of states in the various separations for the bosonic lattices will be different from those for the electronic lattices. By drawing out the lattice diagrams for some sizes in all three dimensions, it is seen that if we denote the total number of states in the various separations by $n_{L_{CB}}$ and the number of nearest neighbours to a site for these separations by $P_{L_{CB}}$, then the total number of states in a separation will be:

$$n_{L_{CB}} = P_{L_{CB}} \text{ x K,} \tag{3.1}$$

where K is as defined earlier.

The $P_{L_{CB}}$ of the various separation of any lattice in all the three dimensions can be obtained from the following rules::

A. For any even 1D lattice, the nearest neighbour (s) for $L_{CB} = 0$ is $P_{L_{CB}} = 1$ while for $L_{CB} > 0$, $P_{L_{CB}} = 1$ except for $L_{CB} = L_L$ in which $P_{L_{CB}} = 1/2$.

For any odd 1D lattice, the nearest neighbour (s) for $L_{CB} = 0$ is $P_{L_{CB}} = 1$ while for all $L_{CB} > 0$, $P_{L_{CB}} = 1$.

B. For any even 2D lattice, the nearest neighbour (s) for $L_{CB} = 0$ is $P_{L_{CB}} = 1$; for $L_{CB} = L_l$, $P_{L_{CB}} = 2$; for $L_{CB} = L_d$, $P_{L_{CB}} = 4$; for $L_{CB} = L_{ld}$, $P_{L_{CB}} = 2$; for $L_{CB} = L_L$, $P_{L_{CB}} = 1$; for $L_{CB} = L_D$, $P_{L_{CB}} = 2$ and for $L_{CB} = L_{LD}$, $P_{L_{CB}} = 1/2$.

For any odd 2D lattice, the nearest neighbour (s) for $L_{CB} = 0$ is $P_{L_{CB}} = 1$; for $L_{CB} = L_l$ and $L_{CB} = L_L$, $P_{L_{CB}} = 2$; for $L_{CB} = L_d$ and $L_{CB} = L_D$, $P_{L_{CB}} = 4$; for $L_{CB} = L_{ld}$ and for $L_{CB} = L_{LD}$, $P_{L_{CB}} = 2$.

C. For any 3D cubic lattice, the nearest neighbour (s) for $L_{CB} = 0$ is $P_{L_{CB}} = 1$; for $L_{CB} = L_l$, $P_{L_{CB}} = 3$; for $L_{CB} = L_d^{2D}$, $P_{L_{CB}} = 12$; for $L_{CB} = L_{ld}^{2D}$, $P_{L_{CB}} = 6$; for $L_{CB} = L_d^{3D}$, $P_{L_{CB}} = 12$ when $x = y \neq z$, $x \neq y = z$ or $x = z \neq y$ and 24 when $x \neq y \neq z$; for $L_{CB} = L_{lD}^{3D}$, $P_{L_{CB}} = 4$; for $L_{CB} = L_L$, $P_{L_{CB}} = 1\,1/2$; for $L_{CB} = L_D^{2D}$, $P_{L_{CB}} 6$; for $L_{CB} = L_{LD}^{2D}$, $P_{L_{CB}} = 1\,1/2$; for $L_{CB} = L_D^{3D}$, $P_{L_{CB}} = 6$ when $x \neq y = z$, $P_{L_{CB}} = 3$ when $x = y \neq z$ and $P_{L_{CB}} = 12$ when $x \neq y \neq z$ and for $L_{CB} = L_{LD}^{3D}$, $P_{L_{CB}} = 1/2$.

For any odd 3D lattice, the nearest neighbour (s) for $L = 0$ is $P_{L_{CB}} = 1$; for $L_{CB} = L_l$ and $L_{CB} = L_L$, $P_{L_{CB}} = 3$; for $L_{CB} = L_d^{2D}$, $P_{L_{CB}} = 12$; for $L_{CB} = L_{ld}^{2D}$, $P_{L_{CB}} = 6$; for $L_{CB} = L_d^{3D}$, $P_{L_{CB}} = 12$ when $x = y \neq z$, $x \neq y = z$ or $x = z \neq y$ and 24 when $x \neq y \neq z$; for $L_{CB} = L_{lD}^{3D}$, $P_{L_{CB}} = 4$; for $L_{CB} = L_D^{2D}$, $P_{L_{CB}} = 12$; for $L_{CB} = L_{LD}^{2D}$, $P_{L_{CB}} = 6$; for $L_{CB} = L_D^{3D}$, $P_{L_{CB}} = 12$ when $x = y \neq z$, $x \neq y = z$ or $x = z \neq y$ and 24 when $x \neq y \neq z$ and for $L_{CB} = L_{LD}^{3D}$, $P_{L_{CB}} = 4$.

By comparing these rules with those for the two electron problem, it is easy to observe that the $P_{L_{CB}}$ is related to that of the electrons, $P_{L_{CE}}$ as follows;

For even 1D lattice, when $L_C = L_L$, $P_{L_{CB}} = P_{L_{CE}}$: when $L_C > 0$, $P_{L_{CB}} = \frac{1}{2}P_{L_{CE}}$ and when $L_C = L_L$ $P_{L_{CB}} = \frac{1}{4}P_{L_{CE}}$.

And for any odd 1D lattice, when $L_C = 0$, $P_{L_{CB}} = P_{L_{CE}}$ while for all $L_{CB} > 0$, $P_{L_{CB}} = \frac{1}{2}P_{L_{CE}}$.

For even 2D and 3D lattices, when $L_C = 0$, $P_{L_{CB}} = P_{L_{CE}}$ while for all $L_C > 0$, $P_{L_{CB}} = \frac{1}{2}P_{L_{CE}}$ except for the longest diagonal length L_{LD} in which $P_{L_{CB}} = 1/4\,P_{L_{CE}}$.

And for odd 2D and 3D lattices, when $L_C = 0$, $P_{L_{CB}} = P_{L_{CE}}$ while for all $L_C > 0$, $P_{L_{CB}} = \frac{1}{2}P_{L_{CE}}$.

Also it is easy to show that like the case of the electrons, the total number of states in a lattice will be

$$\sum P_{L_C} \times K \qquad (3.2)$$

where $P_{L_{CB}} = \frac{K+1}{2}$ for bosons and $P_{L_{CE}} = K$ for electrons.

Eq. (3.2) agrees with Eqs. (2.4) and (2.6) obtained in sec.II for the total number of states for bosons and electrons respectively.

The rules obtained in this sec. are applied to N =1 0, 11, N x N = 10 x 10, 11 x 11 and N x N x N =10 x 10 x 10 and 11 x 11 x 11 and the results shown in Tables I-III.

Table I: A table showing the total number of states in the various separations for even N =10 and odd N = 11.

L_{CB}	$P_{L_{CB}}$ (10)	$n_{L_{CB}}$ (10)	$P_{L_{CB}}$ (11)	$n_{L_{CB}}$ (11)
O	1	10	1	11
1	1	10	1	11
2	1	10	1	11
3	1	10	1	11
4	1	10	1	11
5	1/2	5	1	11
	$\sum P_{L_{CB}} = 5\,1/2$	$\sum n_{L_{CB}} = 55$	$\sum P_{L_{CB}} = 6$	$\sum n_{L_{CB}} = 66$

Table II: A table showing the total number of states in the various separations for even N x N = 10 x 10 and odd N x N = 11 X 11

L_{CB}	$P_{L_{CB}}$ (10^2)	$n_{L_{CB}}$ (10^2)	$P_{L_{CB}}$ $(11^2$	$n_{L_{CB}}$ (11^2)
0	1	100	1	121
1	2	200	2	242
2	2	200	2	242
3	2	200	2	242
4	4	400	4	484
5	2	200	2	242
6	2	200	2	242
7	4	400	4	284
8	4	400	4	484
9	2	200	2	242
10	2	200	2	242
11	4	400	4	484
12	4	400	4	484
13	4	400	4	484
14	2	200	2	242
15	1	100	2	242
16	2	200	2	242
17	2	200	4	484
18	2	200	4	484
19	2	200	4	484
20	1/2	50	2	242
	$\Sigma P_{L_{CB}}$ =50 $^1/_2$	$\Sigma n_{L_{CB}}$ = 5050	$\Sigma P_{L_{CB}}$ = 61	$\Sigma n_{L_{CB}}$ = 7381

Table III: A table showing the total number of states in the various separations for even N x N x N = 10 x 10 x 10 and odd N x N x N= 11 X 11 x11.

L_{CB}	$P_{L_{CB}}$ (10^3)	$n_{L_{CB}}$ (10^3)	$P_{L_{CB}}$ (11^3)	$n_{L_{CB}}$ (11^3)
0	1	1000	1	1331
1	3	3000	3	3993
2	6	6000	6	7986
3	4	4000	4	5324
4	3	3000	3	3993
5	12	12000	12	15972
6	12	12000	12	15972
7	6	6000	6	7986
8	12	12000	12	15972
9	4	4000	4	5324
10	3	3000	3	3993
11	12	12000	12	15972
12	12	12000	12	15972
13	12	12000	12	15972
14	24	24000	24	31944
15	12	12000	12	15972
16	6	6000	6	7986
17	12	12000	12	15972
18	12	12000	12	15972

19	4	4000	4	5324
20	3	3000	3	3993
21	12	12000	12	15972
22	12	12000	12	15972
23	12	12000	12	15972
24	24	24000	24	31944
25	12	12000	12	15972
26	12	12000	12	15972
27	24	24000	24	31944
28	24	24000	24	31944
29	12	12000	12	15972
30	6	6000	6	7986
31	12	12000	12	15972
32	12	12000	12	15972
33	12	12000	12	15972
34	4	4000	4	5324
35	3/2	1500	3	3993
36	6	6000	12	15972
37	6	6000	12	15972
38	6	6000	12	15972
39	12	12000	24	31944
40	6	6000	12	15972
41	6	6000	12	15972
42	12	12000	24	31944
43	12	12000	24	31944
44	6	6000	12	15972
45	6	6000	12	15972
46	12	12000	24	31944
47	12	12000	24	31944
48	12	12000	24	31944
49	6	6000	12	15972
50	3/2	1500	6	7986
51	3	3000	12	15972
52	3	3000	12	15972
53	3	3000	12	15972
54	3	3000	12	15972
55	1/2	500	4	5324
	$\sum^{P_{Lcn}}$ =5001/2	$\sum^{n_{Lcn}}$ =500500	$\sum^{P_{Lcn}}$ = 666	$\sum^{n_{Lcn}}$ = 886446

CONCLUSION

Physicists rarely consider systems of more than two interacting particles, unless they skip directly to infinity (Goldstein 2002). The method we have developed here has extended to bosonic systems our quest for a method to obtain the states of any two particle interactions on any lattice size in all the three dimensions. It will now be straightforward to extend the highly simplified correlated variational approach under the Hubbard Hamiltonian to bosons with some modification of the Hamiltonian. This is expected to provide an insight into the physics of Bose Einstein Condensation. We have commenced such an investigation and a preliminary report is ready (Akpojotor and Ojobor, 2005).

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