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Carrier states in a quantum dot

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Abstract. The ground-state and excited-state wavefunctions for interacting particles confined in a quantum dot are presented within the framework of the Johnson and Payne model. Properly symmetrized spin and spatial parts are laid out.

1. Introduction

Recent progress in nanotechnology has made it possible to fabricate zero-dimensional structures called quantum dots in which a variable number of carriers may be confined [1–7]. These structures provide unique opportunities to study the behaviour of interacting particles in the extreme quantum limit. In practice gated dot devices [4, 6], are the most common. In these devices, it has been shown that the confining potential has nearly circular symmetry despite the square geometry of the gates and the fact that the evolution of the energy levels with increasing magnetic field is similar to that found for a parabolic potential [8, 9]. Graded GaAs/$Ga_{1-x}Al_xAs$ quantum well structures where the confining potential is essentially parabolic have also been fabricated [10]. Johnson and Payne [11–14] have put forward a model that facilitates the theoretical study of these structures.

2. Formulations

In the Johnson and Payne model the carriers are assumed to interact via the potential

$$V(\boldsymbol{r}_i, \boldsymbol{r}_j) = 2V_0 - \frac{1}{2}m^*\Omega^2|\boldsymbol{r}_i - \boldsymbol{r}_j|^2 \tag{1}$$

where $\boldsymbol{r}_i$ and $\boldsymbol{r}_j$ are the coordinates of the ith and jth carriers, V_0 and Ω are constants and m^* is the carrier mass. The confinement is taken to be harmonic with ω_c being the harmonic constant. This leads to the spatial Hamiltonian

$$H_{\text{space}} = \frac{1}{2m^*}\sum_i \boldsymbol{p}_i^2 + \frac{1}{2}m^*\omega_0^2(B)\sum_i |\boldsymbol{r}_i|^2 + \sum_{i<j}\left[2V_0 - \frac{1}{2}m^*\Omega^2|\boldsymbol{r}_i - \boldsymbol{r}_j|^2\right] + \frac{\omega_c}{2}\sum_i L_{i,z}. \tag{2}$$

Here $\omega_0^2(B) = \omega_0^2 + \omega_c^2/4$, $\omega_c = eB/m^*c$, where $\boldsymbol{B}$ is the magnetic field and the z-component of the angular momentum for particle i is given by $L_{i,z} = x_i p_{i,y} - y_i p_{i,x}$. This is second

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quantized into a centre-of-mass part

$$H_{cm} = \left[\hbar\omega_0(B) - \frac{\hbar\omega_c}{2}\right] A^+A_- + \left[\hbar\omega_0(B) + \frac{\hbar\omega_c}{2}\right] B^+B^- + \hbar\omega_0(B) \tag{3}$$

with centre-of-mass coordinates

$$\boldsymbol{R} = (X, Y) = \frac{1}{N}\sum_i \boldsymbol{r}_i \qquad \boldsymbol{P} = (P_X, P_Y) = \sum_i \boldsymbol{p}_i \tag{4}$$

and a relative mode part

$$H_{\text{rel}} = \left[\hbar\omega_0(B) - \frac{\hbar\omega_c}{2}\right] \sum_{i<j} a_{ij}^+ a_{ij}^- + \left[\hbar\omega_0(B) + \frac{\hbar\omega_c}{2}\right] \sum_{i<j} b_{ij}^+ b_{ij}^- + \frac{(N-1)}{2}\hbar\Omega_0 + N(N-1)V_0 \tag{5}$$

with relative coordinates

$$\boldsymbol{r}_{ij} = (x_{ij}, y_{ij}) = \boldsymbol{r}_i - \boldsymbol{r}_j \qquad \boldsymbol{p}_{ij} = (p_{ij,x}, p_{ij,y}) = \boldsymbol{p}_i - \boldsymbol{p}_j. \tag{6}$$

Here (A^+, B^+) are the raising operators and (A^-, B^-) are the lowering operators for the centre-of-mass mode:

$$A^\pm = \left[\frac{1}{4Nm^*\hbar\omega_0(B)}\right]^{1/2} \left[Nm^*\omega_0(B)(X \mp \mathrm{i}Y) \mp \mathrm{i}(P_X \mp P_Y)\right] \tag{7}$$

$$B^\pm = \left[\frac{1}{4Nm^*\hbar\omega_0(B)}\right]^{1/2} \left[Nm^*\omega_0(B)(X \pm \mathrm{i}Y) \mp \mathrm{i}(P_X \pm P_Y)\right]. \tag{8}$$

The (a^+, b^+) and (a^-, b^-) are the raising and lowering operators for the relative mode

$$a_{ij}^\pm = \left[\frac{1}{4Nm^*\hbar\Omega_0}\right]^{1/2} \left[m^*\Omega_0(x_{ij} \mp \mathrm{i}y_{ij}) \mp \mathrm{i}(p_{ij,x} \mp p_{ij,y})\right] \tag{9}$$

$$b_{ij}^\pm = \left[\frac{1}{4Nm^*\hbar\Omega_0}\right]^{1/2} \left[m^*\Omega_0(x_{ij} \pm \mathrm{i}y_{ij}) \mp \mathrm{i}(p_{ij,x} \pm p_{ij,y})\right]. \tag{10}$$

Both the centre-of-mass and relative mode ladder operators satisfy *most* of the usual commutation relations such as $[A^\pm B^\pm] = 0$ or different operators commute, and $[A^-A^+] = 1$. The difference lies in the relative mode ladder operators which do not fully commute among themselves. In particular

$$[a_{ij}^- a_{kl}^+] = [b_{ij}^- b_{kl}^+] = c_{ijkl} \tag{11}$$

where $c_{ijkl} = 2$ if $i = k$ and $j = l$; $c_{ijkl} = -2$ if $i = l$ and $j = k$; $c_{ijkl} = 1$ if $i = k$ or $j = l$; $c_{ijkl} = -1$ if $i = l$ or $j = k$ and $c_{ijkl} = 0$ if $i \neq k, l$ and $j \neq k, l$.

The spin part of the Hamiltonian

$$H_{spin} = -g^*\mu_B B \sum_i s_{i,z} \tag{12}$$

depends on the spin only.

In this paper we shall derive the wavefunctions for the model and in doing so we shall show the existence and location of the spurious states. The essential requirements for the wavefunctions are that they be orthonormal and that they obey the Pauli exclusion principle in the case of a system of a number of fermions. A number of methods exist for the production of many-electron wavefunctions. Most of them work from the combination

of single-electron wavefunctions or single-electron spin orbitals in the form of a Slater determinant. Others rely heavily on group theory and the irreducible representations of the group S_n of all permutations of n objects.

The question we are faced with now is how to represent the eigenstates of the model described previously or what are the wavefunctions. From the theory of a nuclear model in which the nuclear forces were assumed to be Hooke's law forces between nucleons, whose antisymmetric eigenfunctions were calculated by Ingram Block and Yu-Chang Hsieh [15, 16], it was shown that not all mathematically possible eigenstates are the physically plausible ones. In other words spurious states may exist which the Pauli principle does not agree with. The method they employed to generate the wavefunctions is not applicable in this case because the coordinates used are different.

The wavefunction of a single electron is not completely characterized by its wavefunction in coordinate space, that is its orbital, but is essentially represented by a product of its orbital and spin parts. For a system of n electrons this requirement is still needed but the representation of the wavefunction of a many-electron system as a product of the orbital many-electron part and the spin part becomes quite a formidable task as the number of electrons increases. In the case of two electrons, antisymmetric and symmetric spin and orbital parts of the wavefunction may separately be produced with ease.

With the discovery of the quantum Hall effect and the fractional quantum Hall effect and the resulting theoretical investigations [17] conventional ways of representing the many-electron state proved to be inefficient. Laughlin [18, 19] proposed a set of variational wavefunctions in order to represent the highly correlated many-electron phase believed to be present in these regimes; for the ground state he proposed a product of Jastrow functions. In this paper we shall produce exact wavefunctions for the highly correlated system of confined carriers existing in the lower-dimensional structures.

3. The wavefunctions

In the present model the operators are not single-electron operators, but are collective operators which obey bosonic statistics. It is also not possible to form totally antisymmetric products of more then two spins [20]. To obtain properly antisymmetrized wavefunctions for our problem we shall make use of the properties of the symmetry group S_n.

The coordinate wavefunctions for the stationary states of a system of two particles may be either symmetric or antisymmetric under the exchange of the two particles. For a system of an arbitrary number of particles, the coordinate wavefunctions need not necessarily be either symmetric or antisymmetric with respect to the interchange of any pair of particles. It is the complete wavefunction, which includes the spins, which must be symmetric or antisymmetric according to the statistics.

The fact that the particles are identical means that the Hamiltonian is invariant under the interchange of the particles. Hence the wavefunctions obtained from the various interchanges of the variables will also be solutions of the Hamiltonian. In other words H commutes with all permutation operators $\hat{P}$. These operators however do not commute with one another and so they cannot simultaneously be brought into diagonal form. This means that the wavefunctions cannot be so chosen that each of them is either symmetric or antisymmetric with respect to all interchanges separately. From the mathematical point of view, the problem is to find irreducible representations of the permutation group S_n [21].

The method used in producing the wavefunctions for the model strongly relies on the Young diagrams or Young tableaux [21]. The wavefunction for a system of n fermions should belong to the group S_n of all permutations of n objects. The full set of Young

diagrams for the number n of 'objects' represents the standard irreducible representations of the group S_n where the shape of the diagram is in one-to-one correspondence with an irreducible representation of S_n. Thus for $n = 2$ we have figure 1 representing the two irreducible representations of the group.

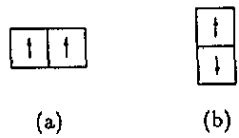

Figure 1. The two spin states for the group S_2: (a) is the $S = 1$ state and (b) is the $S = 0$ spin state.

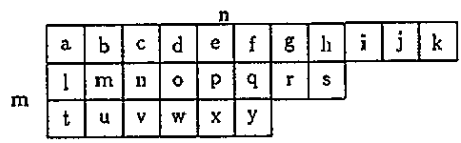

Figure 2. Young tableau containing m rows and n columns which have been labelled in alphabetical order.

The Young tableau represents a function which is initially fully symmetric with respect to interchanges along each row. It is then antisymmetrized with respect to interchanges between two partitions along a column. In the final analysis a Young tableau made up of m rows and n columns will be of mixed symmetry with respect to interchanges along any column or row, except for interchanges between the extra boxes jutting out of the first row from the top which belong to single box columns and will remain fully symmetric. Thus, for the Young tableau depicted in figure 2, particles i, j and k will be symmetric with respect to interchanges within themselves, and all other combinations will be of mixed symmetry.

The $n = 2$ case is special as the irreducible representations are either fully symmetric or fully antisymmetric. The difference starts with the $n = 3$ case where there are three irreducible representations—one fully symmetric, one fully antisymmetric and a third of mixed symmetry, whose Young diagrams are shown in figure 3. The number of irreducible representations for $n = 2$ is 2 and that for $n = 3$ is 3. The dimension for arbitrary n is given by the number of differently shaped Young diagrams. Figure 3 shows the irreducible representations for the case $n = 3$.

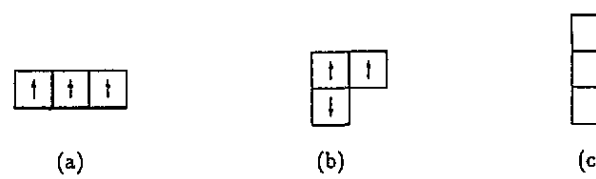

Figure 3. Young diagrams representing the three possible spin states for the case where $N = 3$: (a) is the Young diagram for the $S = 3/2$ spin state and (b) is the Young diagram for the $S = 1/2$ spin state; (c) represents an unacceptable state.

A Young tableau on the other hand is a Young diagram of a given shape which has its boxes numbered in the 'standard' manner [21]. The standard Young tableaux are in one-to-one correspondence with the basis functions for an irreducible representation. Their number therefore gives the dimension for the irreducible representation. This may be illustrated for

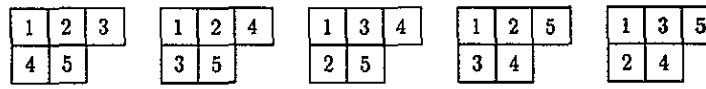

Figure 4. Standard tableaux for the group S_5 for the partition [3, 2].

the case in which $n = 5$, where the Young tableaux are given by figure 4 for the partition [32] (i.e. three boxes in the top row, two in the second and bottom row), which forms one of the classes or irreducible representations for S_n. For each of the standard tableaux in each of the irreducible representations there exists a dual which is given by transposing the columns of the particular tableau. Figure 5 shows the duals for $n = 13$. The summation over the products of each standard Young tableau with its dual represents a function which is fully antisymmetric under any permutation of the coordinates.

We shall now construct antisymmetrized wavefunctions for the model outlined previously using the relative mode operators in doing so and the Young diagrams. One can think of the Young tableau as representing the coordinate wavefunction and its dual the spin function or vice versa for the system of n electrons. This introduces a limit to the number of physically acceptable irreducible representations or shapes of the Young diagrams. As is well known the spin of an electron (or hole) can be in either of two states. Each of the partitions of a particular row of a Young diagram represents a certain state. Therefore the Young diagram representing the spin part of the wavefunction can only have two rows at most. This is depicted in figure 6. The total spin of the above Young tableau is equal to

$$(m - n)/2. \tag{13}$$

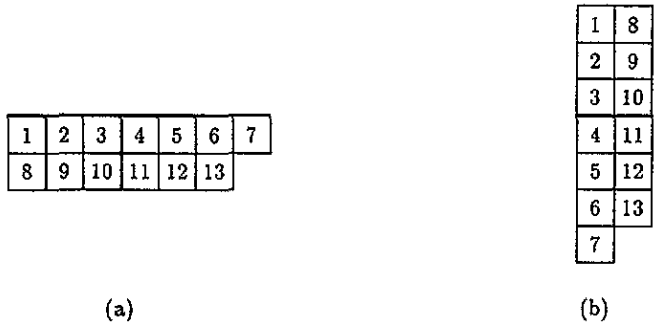

Figure 5. The Young tableau in (a) represents the partition [7, 5] for the group S_{13}. Its dual is shown in (b).

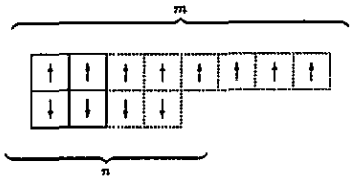

Figure 6. A Young diagram showing the spin state for the partition $[m, n]$ of the group S_{m+n}.

The Young diagrams representing the spatial coordinates of the system are the duals of the spin Young diagrams and can therefore have a maximum of two columns. As has been

shown, totally antisymmetric spin spatial states can be formed from a sum over the products of each one of the spatial basis functions with its dual spin part. By inspection, one may see that the state of highest spin antisymmetry is the lowest-energy state as the spatial function is the most symmetric. This means that the lower S total spin state of the system forms the ground state. The spin Young tableau has to have the maximum number of rows and the minimum number of columns possible. A few examples will serve to clarify this point.

For $N = 2$, only two possible total spin states exist—the $S = 0$ singlet and the $S = 1$ triplet total spin states whose spin Young diagrams are shown in figure 1. The state with $S = 1$ is fully symmetric in spin variables. Its dual is therefore fully antisymmetric in spatial coordinates. The spatial state for the dual of the fully antisymmetric state, $S = 0$, on the other hand, is fully symmetric. Now the 'absolute' ground state for the two-particle system is a spatially fully symmetric state. It is given by the ket $|00\ldots0\rangle$ which, in our model, will be composed of a product of Gaussians and has energy equal to E_g. This forms the true ground state for the two-particle system. The lowest spatially completely antisymmetric state is the $a_{12}^{+}|00\ldots0\rangle$ state as a_{12}^{+} antisymmetrizes the wavefunction. Its energy is higher than E_g by one relative electron–electron mode quantum.

The $N = 3$ spin Young diagrams are given in figures 3(a) and (b). Figure 3(c) is not acceptable as there can only be two spin-half states. The ground state for the 3 particle state cannot therefore be formed from the fully symmetric 'absolute' ground state which is represented by the ket $|00\ldots0\rangle$. The lowest-energy physically acceptable state is the $S = 1/2$ state. Its spatial dual is represented by the same Young diagram and is written as $a_{ij}^{+}|00\ldots0\rangle$ where ij may either be 12, 13 or 23. We will later show how to produce an orthonormal, equally weighted basis using the Young tableaux for a certain Young diagram, and hence how the full wavefunction may be written.

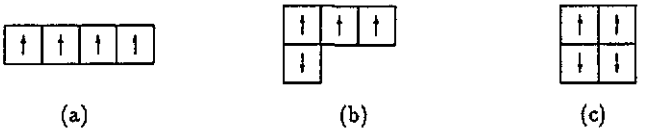

Figure 7. The Young diagram for the three physically acceptable spin states for $N = 4$ fermions: (a) is the spin $S = 2$ state; (b) is the spin $S = 1$ state and (c) is the spin $S = 0$ state.

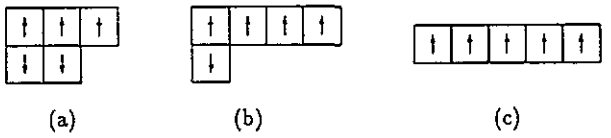

Figure 8. Young diagrams representing the three possible spin states for the case of five fermions: (a) is the $S = 1/2$ ground state; (b) and (c) are the $S = 3/2$ and $5/2$ spin states respectively.

Although the $N = 2$ and $N = 3$ are both two dimensional due to the restrictions imposed by the spin, the $N = 4$ state is seen to be three dimensional with Young diagrams given in figure 7. The three states are composed of the $S = 2$ fully symmetric spin state, and, the $S = 1$ and $S = 0$ mixed-symmetry states. In this case too the ground state is seen not to be the spatially fully symmetric state. Due to the limitation of space we shall not fully investigate all N-particle ground states. It suffices to say that the 'absolute' ground state for an N-fermion system is the lowest total-spin S state and that this may not necessarily be the physically acceptable ground state. The energy is of course an eigenvalue of the spatial

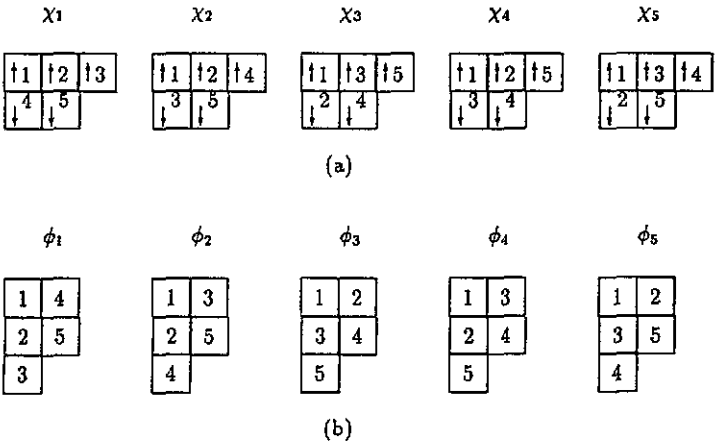

Figure 9. (a) The Young tableaux representing the spin basis functions for the five spin-1/2 fermions for total-spin $S = 1/2$ state. (b) The Young tableaux representing the spatial basis functions for the five spin-1/2 fermions for the total-spin $S = 1/2$ state.

or the dual of the Young diagram for the spin. Let us investigate the state with $N = 5$ particles as this encompasses most of the relevant rules.

It is easier to start with the relevant Young diagrams for the spin and hence produce the spatial ones which form a basis for the wavefunctions. The physically acceptable spin states are properly represented by the appropriate Young diagrams which are given in figure 8 together with their total spins S.

The $N = 5$ case is composed of three allowed spin states. The first is represented by the Young diagram shown in figure 8(a) which has $S = 1/2$ and is of mixed symmetry. This state is five dimensional and forms the ground state. The Young diagram of figure 8(b) represents the spin part of an excited state. This state is also of mixed symmetry. It has a total spin $S = 3/2$ and is four dimensional. The Young diagram for the third state is shown in figure 8(c). This state is only one dimensional with spin $S = 5/2$ and is fully symmetric.

The energy of the ground states is equal to E_g plus five times the relative electron–electron mode quantum. Its basis spin states are represented by the Young tableaux shown in figure 9(a) whose duals which represent their spatial parts are shown in figure 9(b). The set of spatial basis functions $\{\phi_i\}$

$$\phi_1 = a_{12}^+ a_{13}^+ a_{23}^+ a_{45}^+ |00\ldots\rangle \tag{14}$$

$$\phi_2 = a_{12}^+ a_{14}^+ a_{24}^+ a_{35}^+ |00\ldots\rangle \tag{15}$$

$$\phi_3 = a_{13}^+ a_{15}^+ a_{35}^+ a_{24}^+ |00\ldots\rangle \tag{16}$$

$$\phi_4 = a_{12}^+ a_{15}^+ a_{25}^+ a_{34}^+ |00\ldots\rangle \tag{17}$$

$$\phi_5 = a_{13}^+ a_{14}^+ a_{34}^+ a_{25}^+ |00\ldots\rangle \tag{18}$$

are not orthogonal to each other due to the non-trivial commutation relations of the relative mode operators of equations (9) and (10).

The next exercise is to produce the full wavefunction using an orthonormal basis set. This can be done with the help of the Schmidt process [22, 23], which is used to produce

the orthonormal basis set from the set of ϕ_i spatial basis functions. The set of orthonormal basis functions are subsequently obtained as

$$\psi_i = \phi_i - \sum_{j<i} \frac{(\psi_j \phi_i)}{(\psi_j)^2} \psi_j \tag{19}$$

where the brackets signify inner products of the vectors. Hence the full wavefunction is given by $\sum_i \Psi_i \chi_i$ where the set of spinors χ_i are assumed to be orthonormal.

3.1. Example

A simple non-trivial fully worked out example would be the ground state for the three-fermion case (figure 3(b)). The non-orthogonal basis states may be represented by

$$\phi_1 = a_{12}^+ |00..\rangle \tag{20}$$

and

$$\phi_2 = a_{13}^+ |00..\rangle. \tag{21}$$

The orthogonal spatial states can be deduced from the relationships (equation (19))

$$\psi_1 = a_{12}^+ |00..\rangle \tag{22}$$

and

$$\psi_2 = a_{13}^+ |00..\rangle - \frac{\langle a_{12}^- a_{13}^+ \rangle}{\langle a_{12}^- a_{12}^+ \rangle^2} |a_{12}^+\rangle \tag{23}$$

where the inner brackets are simply worked out from the commutators giving

$$\langle a_{12}^- a_{13}^+ \rangle = \langle ([a_{12}^- a_{13}^+] + a_{13}^+ a_{12}^-) \rangle = [a_{12}^- a_{13}^+] = 1 \tag{24}$$

and

$$\langle a_{12}^- a_{12}^+ \rangle^2 = 4 \tag{25}$$

and hence

$$\psi_2 = a_{13}^+ |00..\rangle - \frac{1}{4} a_{12}^+ |00..\rangle. \tag{26}$$

The case where $N = 5$ is also solvable but is more tedious with the inner products $\langle \psi_i \phi_j \rangle$ deduced from the commutators which have $s!$ terms where s is the number of ladder operators in ϕ_i.

4. Conclusion

In this paper we have outlined a method for generating the wavefunctions which obey the proper symmetry conditions for any number of particles interacting via Hooke's law forces. In doing so we have managed to locate the spurious states and therefore the mathematical ground state energies which are not physically acceptable. We can therefore now generate the eigenenergies for the system.

The case of $N = 3$ was explicitly investigated in order to show the method by which an orthonormal basis set may be generated. We have also touched upon the three-fermion case in order to give a complete example. Although it was not dwelt upon, a basis set which is not orthonormal would not represent the N particles properly so that they are all antisymmetric under any exchange. Due to the limitation of space we shall be unable to give any more specific examples of the use of the method for generating the wavefunctions for the system.

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