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EXACT RESULTS FOR A SYSTEM OF INTERACTING ELECTRONS IN ONE-DIMENSIONAL CONFINEMENTS

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Abstract: We study the ground state behavior/properties of a system of interacting electrons confined one-dimensionally. To describe the system, we first derive a set of fundamental equations with the aid of the Bethe ansatz method. We then obtain an exact numerical solution for this set of fundamental equations to determine the ground state energy/properties for a few electrons inside a one-dimensional confinement. On the basis of the obtained results, we discuss the effects of the electron-electron interaction on the ground state properties of the system of interacting electrons confined in one-dimension. We also compare the results derived by imposing periodic boundary conditions, to those derived by imposing that the electrons are (one dimensionally) confined by infinitely high potential walls (hard walls). From these results, we can conclude that a proper description of the boundary conditions is indeed necessary for a correct estimation of the effect of the electron-electron interaction.

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This should lead us to a correct interpretation of the electron dynamics, and proper evaluation of the functionalities of novel materials based on this system.

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1. Introduction

Recent advances in experimental techniques have enabled us to actually manipulate atoms one-by-one, e.g. with the aid of a scanning tunnelling microscope (STM). This, in turn, makes fabrication of artificial nano-structures, e.g. nanowires and quantum dots, on solid surfaces feasible. The corresponding electron systems in such nano-structures are considered as typical examples of confined quasi-one-dimensional systems of interacting electrons. A knowledge of the general physical properties of such systems is necessary for the realization of real-life application/utilization of such nano-structures. In line with this, we investigate the ground state properties of a system of N interacting electrons confined in a one-dimensional region of length L. Each electron is then referenced by its coordinate $x_i : [0, L]$, where $i = 1, 2, \cdots, N$. We compare the results derived by imposing that the one dimensional confinement is bordered by infinitely high potential walls [1], to those obtained by imposing periodic boundary conditions [2].

2. Model

Consider a system of N electrons in a one-dimensional confinement of length L. Let us denote the correlation between any two electrons in the system by a δ-function type interaction. Let us also assume that the confinement is bordered by an infinitely high potential wall—hard walls. The corresponding Hamiltonian [3], [2], [4], [1] describing the system can then be expressed as

$$H = -\frac{\hbar^2}{2m}\sum_i \frac{\partial^2}{\partial x_i^2} + 4u\sum_{i<j}\delta(x_i - x_j), \quad u > 0. \tag{1}$$

$\hbar$ is the Dirac's constant, m gives the electron mass, $u(> 0\ )$ is the (repulsive) Coulomb interaction between two electrons. We want to determine the wave

function (eigenfunction) Ψ that would satisfy the Schrödinger equation (second-order differential equation, second-order eigenvalue equation)

$$H\Psi = E\Psi \tag{2}$$

corresponding to the ground state energy (eigenvalue) E.

Assuming Bethe's hypothesis to be valid [3], we define the corresponding wave function for N electrons in the configuration $Q:\ 0 \le x_{Q_1} < x_{Q_2} < \cdots < x_{Q_N} \le L$ as

$$\Psi^Q = \sum_{\{\tilde{k}\},P} a(Q,P|\{\tilde{k}\}) \exp(\mathrm{i}\sum_{j=1}^{N} \tilde{k}_{P_j} x_{Q_j}), \quad \mathrm{i} = \sqrt{-1}. \tag{3}$$

$P = [P_1, \cdots, P_N]$ and $Q = [Q_1, \cdots, Q_N]$ are two permutations of the integers $1, 2, \cdots, N$. To take into account the electrons scattered back by the infinitely high potential walls at the boundaries, we need to consider N-electron wave functions with corresponding wave numbers $\tilde{k}_j$, which takes both positive and negative values. Thus, $a(Q,P|\{\tilde{k}\})$ in equation (3) is a set of $N! \times N! \times 2^N$ coefficients to be determined for the N-electron system.

Let us consider two configurations. Let one configuration be given by $Q:\ 0 \le x_{Q_1} < x_{Q_2} < \cdots < x_{Q_a} < x_{Q_b} < \cdots < x_{Q_N} \le L$. Let the other configuration Q' be such that the coordinates of the Q_a-th and Q_b-th electrons are interchanged., i.e. $Q':\ 0 \le x_{Q_1} < x_{Q_2} < \cdots < x_{Q_b} < x_{Q_a} < \cdots < x_{Q_N} \le L$. To satisfy the continuity of Ψ and the proper discontinuity of its first derivative at $x_{Q_a} = x_{Q_b}$, as required by equation (2), it is sufficient to have

$$a(Q,P'|\{\tilde{k}\}) = Y_{ij}^{ab} a(Q,P|\{\tilde{k}\}), \tag{4}$$

where

$$P, P':\ p_1 = p'_1,\ \cdots, p_a = i = p'_b,\ p_b = j = p'_a,\ \cdots, p_N = p'_N. \tag{5}$$

The operator Y is defined by

$$Y_{ij}^{ab} = \left[\frac{\hbar^2}{2m}\left(\tilde{k}_i - \tilde{k}_j\right) P_{ab} - 2ui\right] \Big/ \left[\frac{\hbar^2}{2m}\left(\tilde{k}_i - \tilde{k}_j\right) + 2ui\right], \tag{6}$$

where

$$\tilde{k}_{-i} = -\tilde{k}_i, \tag{7}$$

and P_{ab} is a permutation operator which exchanges the coordinates of Q_a and Q_b. The operator Y_{ij}^{ab} satisfies the Yang-Baxter equation [2].

Imposing the boundary condition $\Psi(x_1, \cdots, x_j = 0, \cdots, x_N) = 0$ and $\Psi(x_1, \cdots, x_j = L, \cdots, x_N) = 0$, we get

$$X^{1,j}_{1,j} X^{2,j}_{2,j} \cdots X^{j-1,j}_{j-1,j} a^I_j + X^{1,j}_{1,-j} X^{2,j}_{2,-j} \cdots X^{j-1,j}_{j-1,-j} a^I_{-j} = 0\,, \tag{8}$$

and

$$e^{i\tilde{k}_j L} X^{j,N}_{j,N} X^{j,N-1}_{j,N-1} \cdots X^{j,j+1}_{j,j+1} a^I_j + e^{-i\tilde{k}_j L} X^{j,N}_{-j,N} X^{j,N-1}_{-j,N-1} \cdots X^{j,j+1}_{-j,j+1} a^I_{-j} = 0, \tag{9}$$

where I is the identity operator. Here X^{ab}_{ij} is an operator that exchanges the electron with wave number $\tilde{k}_i$ at $x = x_{Q_a}$ and the electron with $\tilde{k}_j$ at $x = x_{Q_b}$, and is defined by

$$X^{ab}_{ij} = P_{ab} Y^{ab}_{ij} = \left[\frac{\hbar^2}{2m}\left(\tilde{k}_i - \tilde{k}_j\right) - 2uiP_{ab}\right] \Big/ \left[\frac{\hbar^2}{2m}\left(\tilde{k}_i - \tilde{k}_j\right) + 2ui\right]. \tag{10}$$

From equation (8) and equation (9), we derive the following relation:

$$(X^{j,j+1}_{j+1,j} \cdots X^{j,N}_{N,j})(X^{j,N}_{-j,N} \cdots X^{j,j+1}_{-j,j+1}) \times (X^{j-1,j}_{-j,j-1} \cdots X^{1,j}_{-j,1})(X^{1,j}_{1,j} \cdots X^{j-1,j}_{j-1,j}) a^I_j = e^{2i\tilde{k}L} a^I_j. \tag{11}$$

3. Results and Discussion

We can now solve equation (11) for $\{\tilde{k}\}$ and, determine the coefficients from equations (4), (8), and (9). Here, let us first consider the case of $N = 2$ electrons. In Figure 1, we show the ground state energy $E = \frac{\hbar^2}{2m}(\tilde{k}_1^2 + \tilde{k}_2^2)$ as a function of the electron-electron interaction u, calculated by imposing that the one dimensional confinement is bounded by hard walls (Figure 1(a)), or periodic boundary conditions (Figure 1(b)). We see that as we increase u, the corresponding ground state energy of a singlet state [5] approaches an asymptotic value that corresponds to the ground state energy of the triplet states [5]. Also note that the ground state energies derived by imposing that the one dimensional confinement is bounded by hard walls are larger than those derived using periodic boundary conditions.

In Figure 2 we show the corresponding spatial distribution of the $N = 2$ electrons. As we gradually increase u, the corresponding spatial distribution

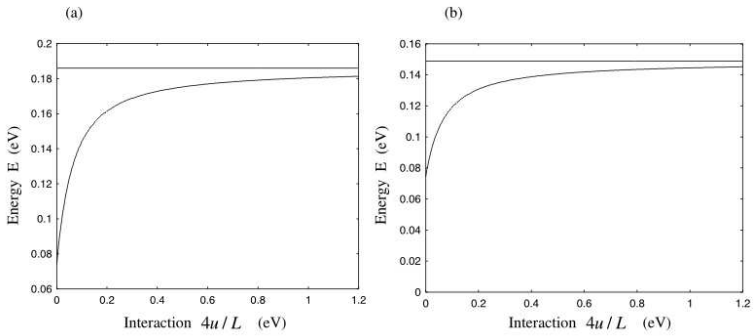

Figure 1: The ground state energy of $N = 2$ electrons in a one-dimensional confinement of length $L = 3.18$ (nm), as a function of the electron-electron interaction $4.0u/L$ (eV), calculated by imposing (a) that the one dimensional confinement is bounded by hard walls, or (b) periodic boundary conditions.

of the two electrons bounded by hard walls (Figures 2(a), (c) and (e)) shows a gradual but continuous change from one corresponding to two non-interacting electrons (for $u = 0$), to that of a triplet state case, where the two electrons completely avoid each other. For the solutions under periodic boundaries (Figures 2(b), (d) and (f)), the corresponding spatial distribution of the electrons also shows a gradual change. We note that under periodic boundaries, the two electrons are most likely distributed spatially in such a way that their coordinates satisfy the following relation: $|x_1 - x_2| = L/2$ for $u \neq 0$ because the i-th electron at $x = x_i$ interacts with the j-th electrons which exists both at $x = x_j$ and $x = x_j \pm L$.

Next, let us consider the case where there are $N = 3$ electrons in the confinement. We transform the wave functions in equation (11) from coordinate space to spin [5] space Ψ_σ [1]:

$$(X_{j+1,j}^{j,j+1^\sigma} \cdots X_{N,j}^{j,N^\sigma})(X_{-j,N}^{j,N^\sigma} \cdots X_{-j,j+1}^{j,j+1^\sigma}) \times (X_{-j,j-1}^{j-1,j^\sigma} \cdots X_{-j,1}^{1,j^\sigma})(X_{1,j}^{1,j^\sigma} \cdots X_{j-1,j}^{j-1,j^\sigma})\Psi_\sigma = e^{2i\tilde{k}_j L}\Psi_\sigma. \quad (12)$$

Here the operator X^σ is defined by

$$X_{i,j}^{a,b^\sigma} = \left[\frac{\hbar^2}{2m}\left(\tilde{k}_i - \tilde{k}_j\right) + 2uiP_{ab}{}^\sigma\right] \Big/ \left[\frac{\hbar^2}{2m}\left(\tilde{k}_i - \tilde{k}_j\right) + 2ui\right], \quad (13)$$

where $P_{ab}{}^\sigma$ is an operator which exchanges spin coordinates, and Ψ_σ is the spin eigenfunction. Again, we solve equation (12) for $\{\tilde{k}\}$ and, from equations

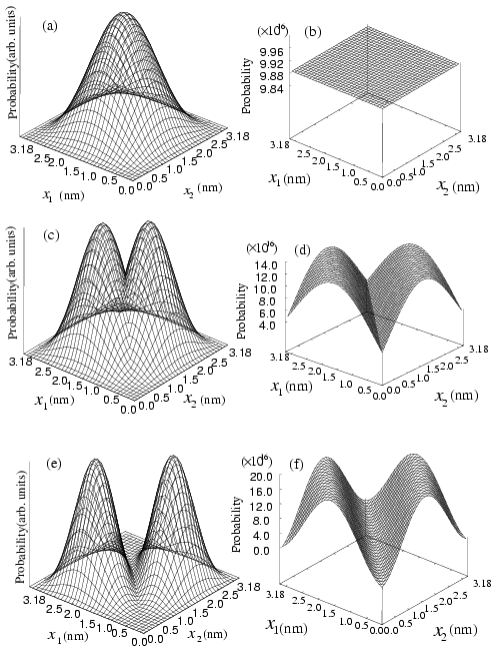

Figure 2: Spatial distribution of the $N = 2$ electrons in a one-dimensional confinement of length $L = 3.18$ (nm), when $4.0u/L =$ (a), (b) 0.0 (eV), (c), (d) 0.04 (eV) and (e), (f) 0.4 (eV), in the singlet state. Results shown in (a), (c), (e) are calculated by imposing that the one dimensional confinement is bounded by hard walls, whereas those in (b), (d), (f) are calculated by imposing periodic boundary conditions.

(4), (8), and (9), we can determine the coefficients for the case when there are now $N = 3$ electrons. We show the calculated spatial distribution of the $N = 3$ electrons in Figure 3. We assume that the spins of the 1-st, 2-nd, and 3-rd electrons are up, down and up respectively. We also assume that the 2-nd electron is fixed at $x = L/2$. When the electron-electron interaction $4.0u/L = 0.4$(eV) (Figure 3(a)), we find the 1-st and 3-rd electrons at either sides (e.g. $0 < x_1 < L/2 < x_3 < L$ or $0 < x_3 < L/2 < x_1 < L$) of where the 2-nd electron, with a down spin, is (i.e. at $x = L/2$). We also see that there is, however, a very slight possibility of finding both the 1-st and 3-rd electrons, at same side of the 2-nd electron (e.g. $0 < x_1, x_3 < L/2$ or $L/2 < x_1, x_3 < L$). Regardless of the conditions, however, both electrons try to stay as far from

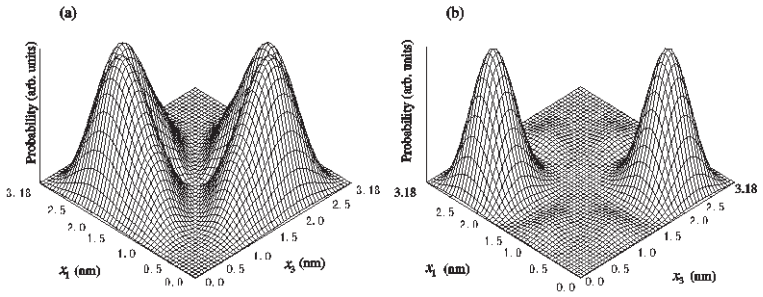

Figure 3: Ground state spatial distribution of the electron density of $N = 3$ electrons in one-dimensional confinement of length $L = 3.18$ (nm), when $4.0u/L =$ (a) 0.4 (eV) and (b) 4.0 (eV), calculated by imposing that the one dimensional confinement is bounded by hard walls. We assume that the spins of the 1-st, 2-nd, and 3-rd electrons are up, down and up respectively. We also assume that the 2-nd electron is fixed at $x = L/2$.

$x = L/2$, as much as possible. When $4.0u/L = 4.0$(eV) (Figure 3(b)), the $N = 3$ electrons completely avoid each other, and we never find both the 1-st and 3-rd electrons at the same side of the 2-nd electron.

4. Summary

In conclusion, we derive a set of fundamental equations, explicitly taking into account the confinement of the system. We then obtain the exact numerical solution of this set of fundamental equations to determine the ground state energy/properties for a few electrons in the system. On the basis of the obtained results, we discuss the effects of the confinement and the electron-electron interaction on the ground state properties of the system of interacting electrons confined in one-dimension, comparing the results of the case of periodic boundaries. From these results, we can conclude that a proper description of the boundary conditions is indeed necessary for a correct estimation of the effect of the electron-electron interaction. This should lead us to a correct interpretation of the electron dynamics, and proper evaluation of the functionalities of novel materials based on this system of N-bodies (electrons) in a finite confinement.

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References

[1] K. Tsujimoto, H. Kasai, W.A. Diño, H. Nakanishi, A. Okiji, Some solutions for a system of interacting electrons confined in one dimension, *Physics Letters*, **A277** (2000), 123-128.

[2] C.N. Yang, Some Exact results for the many-body problem in one dimension with repulsive delta-function interaction, *Physical Review Letters*, **19** (1967), 1312-1315.

[3] C.N. Yang, C.P. Yang, One-dimensional chain of anisotropic spin-spin interaction. I. Proof of Bethe's hypothesis for ground state in a finite system, *Physical Review*, **50** (1966) 321-327.

[4] H. Schulz, Hubbard chain with reflecting ends, *Journal of Physics C: Solid State Physics*, **C18** (1985), 581-601.

Note. Electrons are negatively charged particles found in an atom. Along with neutrons and protons, they comprise the building blocks of all atoms. In addition to its charge, an electron has an instrinsic property called spin $|s| = 1/2$, with a magnetic moment associated to it. Thus, we could consider, e.g. an upright bar magnet with the North pole pointing up, as analogous to an electron with spin up $s = +1/2$. A spin down electron $s = -1/2$ would be analogous to an upright bar magnet with the North pole pointing down. As with bar magnets, bringing together two spin up or two spin down electrons requires

a much higher energy than that required to bring two electrons of opposite spins. Two electrons with opposite spins have a total spin $|S| = |s_1 + s_2| = 0$, and they form a singlet state. Adding another electron, the total spin $|S| = |s_1 + s_2 + s_3| = |s_1 - s_1 + s_3| = 1/2$, forming a doublet state. Two electrons with the same spin have $|S| = |s_1 + s_2| = 1$, and they form a triplet state. In general, N electrons with total spin $|S| = |s_1 + s_2 + \cdots + s_N|$ form a $|2S + 1|$-tuplet state.