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Energy-Level Structure of a Confined Electron-Positron Pair in Nanostructure

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***Abstract*—**The energy-level structure of a pair of electron and positron confined in a quasi-one-dimensional nano-scale potential well has been investigated focusing on its trend in the small limit of confinement strength ω, namely, the Wigner molecular regime. An anisotropic Gaussian-type basis functions supplemented by high angular momentum functions as large as $l = 19$ has been used to obtain reliable full configuration interaction (FCI) wave functions. The resultant energy spectrum shows a band structure characterized by ω for the large ω regime whereas for the small ω regime it shows an energy-level pattern dominated by excitation into the in-phase motion of the two particles. The observed trend has been rationalized on the basis of the nodal patterns of the FCI wave functions.

***Keywords*—**Confined systems, positron, wave function, Wigner molecule, quantum dots.

I. Introduction

RECENT advances in semiconductor technology allows us to fabricate nano-sized objects in which a small number of electrons are confined in artificially designed low-dimensional potential wells. These confined electron systems, referred to as quantum dots or *artificial atoms* [1]-[3], have been studied intensively in the last decade because of their potential applicability for quantum computers, quantum cryptography, or quantum-dot lasers.

The energy-level structure of the quantum dots is known to change strongly for different strength of confinement in accord with the strong variation in the relative importance of the one-electron vs. two-electron operators [4]. For understanding this complicated energy-level structure of artificial atoms in a unified way we have investigated in our previous studies the energy spectra of quasi-two- and quasi-one-dimensional artificial atoms with a few number of electrons ($N = 2 \sim 4$) in detail and have shown that their energy-level patterns can be characterized by the so-called *polyad quantum numbers* for all regimes of the strength of confinement ω [5]-[9]. It was also shown in this course of studies that the quasi-one-dimensional quantum dots are particularly interesting because of an appearance of the so-called *Wigner lattice* or *Winger molecular states* in the weak limit of confinement [10].

On the one hand, recent development in experimental techniques to produce and manipulate antiparticles has triggered studies in the rapidly growing field of *exotic atoms and molecules* that contains a few number of anti-particles, such as a positron, for the most common example, in atoms and molecules. These new systems could be a new source for understanding the nature of confined quantum systems as well as matter-antimatter interaction.

In the present study we have investigated the most simple confined matter-antimatter system, namely, a pair of electron and positron that is confined in a quasi-one-dimensional nanostructure. We have particularly focused on the energy-level structure in the weak limit of confinement and examined if there appears a new type of quantum state analogous to the Wigner molecular state. Atomic units have been used throughout this paper.

II. Theoretical Model and Computational Method

The Hamiltonian for the quasi-one-dimensional two-electron quantum dot and that for the quasi-one-dimensional electron-positron quantum dot have the following respective forms,

$$\hat{H}_{ee} = -\tfrac{1}{2}\sum_{i=1}^{2}\nabla_i^2 + \tfrac{1}{2}\sum_{i=1}^{2}[\omega_z^2 z_i^2 + \omega_{xy}^2(x_i^2 + y_i^2)] + \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \quad (1)$$

$$\hat{H}_{ep} = -\tfrac{1}{2}\sum_{i=1}^{2}\nabla_i^2 + \tfrac{1}{2}\sum_{i=1}^{2}[\omega_z^2 z_i^2 + \omega_{xy}^2(x_i^2 + y_i^2)] - \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \quad (2)$$

where $\boldsymbol{r}_i = (x_i, y_i, z_i)$ for i=1,2, whereas ω_z and ω_{xy} represent the strength of confinement along the z and xy coordinates, respectively. Thanks to the identity between electron and positron except for their sign of charge, the only difference in the Hamiltonians between the electron-electron and electron-positron pairs [(1) and (2), respectively] is the sign in front of the two-particle potentials.

In the above equations the so-called *effective atomic units* have been adopted in which the reduced Planck constant $\hbar$, elementary charge e, effective mass of electron m_e, and effective Coulomb's constant in the matter $1/4\pi\varepsilon^*$, are all set to unity. In the case of GaAs quantum dots, for example, this definition gives one unit of length (effective Bohr radius a_0^*) and energy (effective Hartree energy E_h^*) being equal to 9.79 nm and 11.9 meV, respectively [11]-[12].

For a sufficiently large value of ω_{xy} with respect to ω_z the two particles in the systems are strongly confined in the xy

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directions and can have degrees of freedom only in the z direction. In the present study the value ofω_z is varied in the range between 0.1 and 10.Since the result of calculation is not qualitatively different for different values ofω_{xy} on condition that $\omega_{xy}>>\omega_z$, the value of ω_{xy} is chosen arbitrarily such as 200 and is not explicitly noted hereafter.

Cartesian *anisotropic* Gaussian-type functions [13]-[15] of the form

$$\chi^{\mathbf{a},\xi}(\mathbf{r}) = x^{a_x} y^{a_y} z^{a_z} \exp[-\xi_x x^2 - \xi_y y^2 - \xi_z z^2] \qquad (3)$$

have been used to expand the one-electron orbitals for the Hamiltonians (1) and (2). Following the quantum chemical convention these functions are classified as *s*-, *p*-, *d*-type, etc. for $l = a_x+a_y+a_z = 0$, 1, 2, etc., respectively.

In our previous studies a basis set having one function for each angular momentum shell, i.e., a [1*s*1*p*1*d*1*f*1*g*…] basis set with large angular momentum functions such as $l \geq 10$, was shown to give accurate and reliable results for quasi-one-dimensional quantum dots unless their exponents [ξ in (3)] are properly chosen [7]-[8].

The exponents of these basis functions for two-electron quantum dots have been chosen to be half of ω_z for ξ_z and half of ω_{xy} for ξ_x and ξ_y. Since ω_{xy} is at least 20 times larger than ω_z only functions with $a_x=a_y=0$ have been selected and used in the basis sets. In case of the electron-electron pair the maximum l value in the basis set is chosen as 14 whereas in case of the electron-positron pair it is chosen as large as 19 so as to take care of contraction of the electron and positron density distributions due to their mutual attraction. The eigenfunctions and the corresponding energies for the relevant states have been obtained by diagonalising the full configuration interaction (FCI) Hamiltonian matrix.

III. Results and Discussion

A. Energy Spectra and Two-Particle Wave Functions

The energy spectra of low-lying states of a pair of electron and positron confined in a quasi-one-dimensional harmonic-oscillator potential has been calculated and are plotted in Fig. 1 for ω_z= 10, 4, and 1. In the same figure the two-particle wave functions of the corresponding states projected onto the z_1–z_2 plane have been also displayed where the z_1 and z_2 are either the z coordinates of electron or positron, respectively. Unlike the case of two electron quantum dots, namely, a pair of two electrons confined in quasi-one-dimensional harmonic-oscillator potentials, examined in an earlier study [7], different spin states, singlet and triplet, are always degenerate in the case of the electron-positron pair, since Pauli principle for indistinguishable particles is not applied in this case. Therefore, the label for spin multiplicity is omitted in the assignments of the states given in Fig. 1.

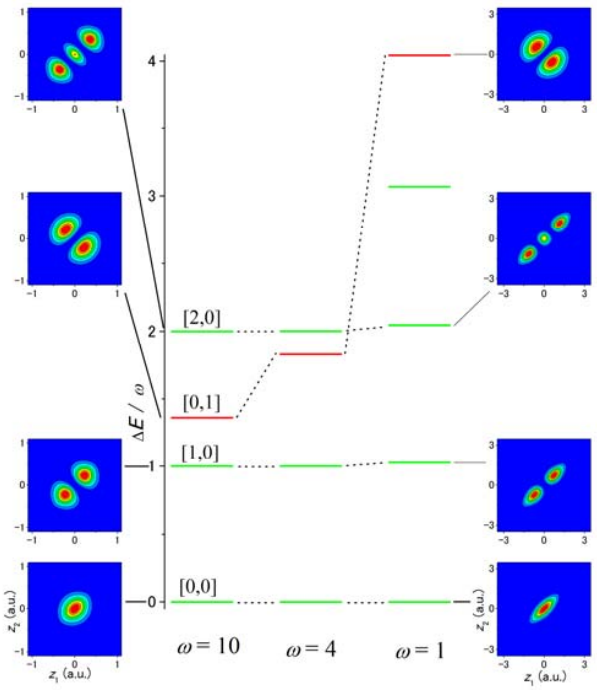

Fig. 1 Correspondence of the low-lying energy levels and wave functions of a pair of electron and positron confined in a quasi-one-dimensional harmonic potential. The vertical axis for all three energy diagrams is divided by ω_z so that the excitation energy of one quantum of ω_z are on the same level. The two-particle wave functions are plotted as the square density in the z coordinates (in a.u.) of electron and positron, z_1 and z_2, respectively

Assignments of quantum numbers to the wave functions of ω_z = 10 displayed in Fig. 1 are made by counting the number of nodes along the *normal-mode* coordinates [6]-[8] in the wave functions. An illustrative example for the correspondence between the wave functions and their assignments is given in Fig. 2. Two types of normal-mode coordinates are indicated by dotted orange lines in Fig. 2 (a): one is the line starting from the left and bottom end towards the upper and right corner, which is called the *symmetric-stretch* normal-mode coordinate, $z_{\text{sym}} \equiv (z_1 + z_2)/\sqrt{2}$, whereas the line orthogonal to it is called the *antisymmetric-stretch* normal-mode coordinate, $z_{\text{asym}} \equiv (z_1 - z_2)/\sqrt{2}$. As their names indicate, the symmetric-stretch coordinate represents the coordinate along which the two particles undergo in-phase motion, whereas the antisymmetric one represents the coordinate along which they undergo out-of-phase motion, respectively. It is noted that this symmetric-stretch normal-mode coordinate is parallel to the *center-of-mass* coordinate.

The wave function (a) in Fig. 2 has one and four nodes along the symmetric-stretch and antisymmetric-stretch coordinates, respectively. Therefore, this wave function can be characterized by a set of two quantum numbers, $[v_s,v_a] = [1,4]$, where v_s and v_a represent the number of nodes along the symmetric-stretch and antisymmetric-stretch coordinates, respectively. In the case of the wave function (b) it has two and

three nodes along the symmetric- and antisymmetric-stretch coordinates, respectively. Therefore, this wave function represents the state with an assignment [2], [3]. Similar arguments can be made to the assignment of quantum numbers to the wave functions of ω_z =10 in Fig. 1.

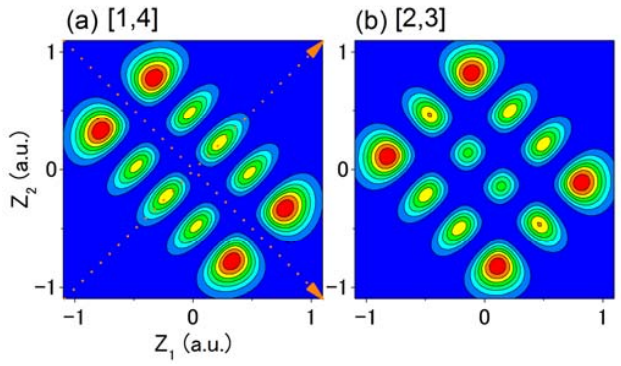

Fig. 2 An illustrative example of the correspondence between the nodal patterns in the two-particle wave functions and their assignments The contour plots (a)and (b) represent, respectively, the probability density distributions of the wave functions for the [1,4] state and the [2,3] state projected onto the z_1–z_2 coordinate space. The dotted orange lines represent the *normal-mode* coordinates of a pair of two particles confined in an one-dimensional space: the diagonal line starting from the left and bottom end and pointing to the upper-right corner represents the symmetric-stretch normal-mode coordinate, whereas the line orthogonal to it the antisymmetric-stretch normal-mode coordinate (See text)

The energy-level structure for large values of ω_z, such as ω_z= 10 as displayed in Fig. 1, is similar to that of the pair of two electrons displayed in Fig. 1 of [7] except for the reversed ordering of the two states, [1,0] and [0,1], that correspond to the ^{1}[1,0] and ^{3}[0,1] states of two electrons, respectively. In this large regime of$\omega_z$the dominance of the harmonic-oscillator confining potential over the inter-particle interaction explains their similarity.

The reversed order of the [1,0] and [0,1] states is caused by the attractive nature of the inter-particle interaction. As displayed in Fig. 1, the probability density distribution of the [0,1] state has a node on the line where z_{asym} = 0 whereas that of the [1,0] state does not. Since the inter-particle interaction is attractive for the positron-electron pair in contrast to the electron-electron pair, the nonzero probability density at z_{asym} = 0 makes the [1,0] state to have a lower energy than the [0,1] state.

The ω_z-scaled excitation energy $\Delta E/\omega_z$ for the [1,0]and [2,0] states is almost constant irrespective of ω_z with the values 1 and 2, respectively. This is a consequence of the *generalized Kohn theorem* [16] as has been observed for the pair of two electrons. Since the Hamiltonian of (2) for the positron-electron pair is also separable with respect to the z_{sym} and z_{asym} coordinates as for the electron-electron pair of (1) and since these [1,0] and [2,0] states have an excitation of one and two quanta, respectively, into the symmetric-stretch mode, namely, *the center-of-mass mode*, the excitation energy from the ground state should be equal to one and two times of ω_z, respectively.

A small deviation of $\Delta E/\omega_z$ for these states from 1 and 2, respectively, for decreasing ω_z is caused by insufficiency of the employed basis set. As seen in the plots of the wave functions for ω_z = 1 in Fig. 1, the probability density distribution is strongly compressed along the z_{asym} axis owing to the strongly attractive positron-electron interaction potential that diverges to $-\infty$ at z_{asym} = 0. As ω_z decreases the positron-electron interaction potential increasingly dominates the total energy over the one-particle confining potential. Therefore, a computational methodology based on one-particle orbitals as commonly used in standard quantum chemical approaches becomes increasingly worse even though the present basis set includes functions having a large number of nodes, as many as, such as 19.

B. Weak Limit of Confinement

The variation of the energy-level structure of the confined positron-electron pair for decreasing ω_z shows a distinct trend than does the confined electron pair. First, in the case of the electron pair the energy levels tend to form degenerate pairs of singlet and triplet states for decreasing ω_z (formation of Wigner molecule) as has been observed in [7], whereas those of the positron-electron pair in the present study do not. Second, in the case of the electron-electron pair the energy levels of those states having excitations into the antisymmetric-stretch mode, such as the [0,1] state, get stabilized, whereas the energy levels of the corresponding states in the positron-electron pair instead increases rapidly as ω_z decreases as displayed in Fig. 1. These distinct trends in the variation of the energy-level structure for the small regime of ω_z can be rationalized as follows.

As ω_z decreases, the magnitude of the positron-electron interaction becomes effectively larger as for the electron pair. Since the two-particle wave functions of those states having excitations only into the symmetric-stretch mode, such as [n,0] (n=1,2, …), have nonzero probability density at z_{asym} = 0, their energy levels get stabilized thanks to the strong positron-electron attraction that diverges to $-\infty$at z_{asym} = 0. On the other hand, since the wave functions of those states having excitations of odd quanta into the antisymmetric-stretch mode have a node at z_{asym} = 0, these states can hardly get a benefit of the energy-lowering by the positron-electron attraction.

The electron density distributions of the four lowest states at ω_z = 10 and those of the corresponding states at ω_z = 1 are displayed in Fig. 3. The electron density distributions of the ground [0,0] state for ω_z = 10 and 1 look quite similar to each other except that the distribution for ω_z = 1 is narrower than for ω_z = 10. This observation is in contrast to the electron pair where the distribution of the ground state is a single maximum for large ω_z but a double maximum for small ω_z[7]. In case of the [1,0] and [2,0] states the nodal structure of the electron density distributions gets increasingly enhanced as ω_z decreases as observed for the electron pair. However, in case of the electron pair the emergence of clear nodal structure in the electron density distributions indicates a signature of formation of Wigner molecule states whereas in case of the positron-electron pair the emergence of a similar nodal

structure *does not* mean Wigner molecule states but a preference of excitations into the symmetric-stretch mode.

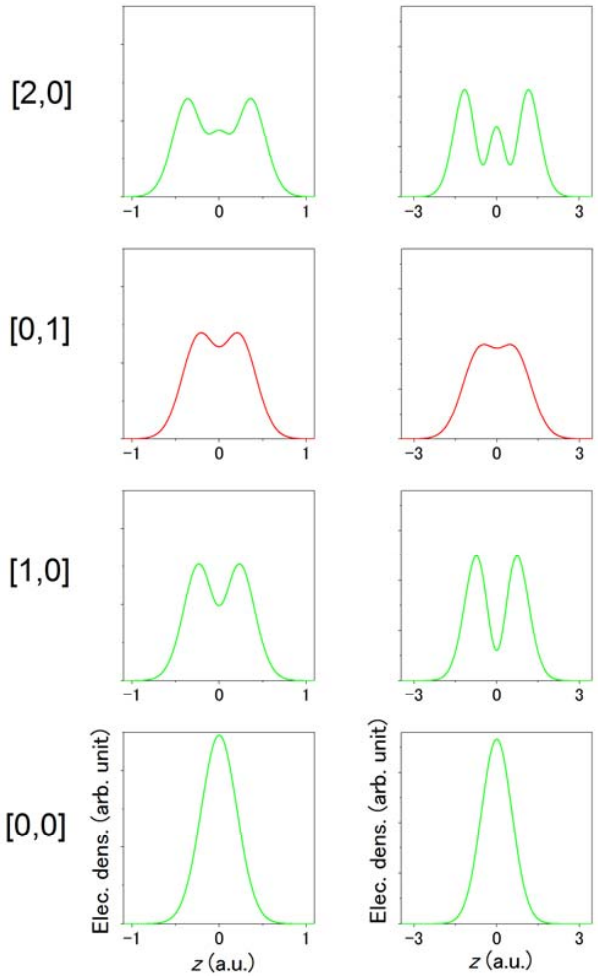

Fig. 3 Electron density distribution of a pair of electron and positron confined in a quasi-one-dimensional harmonic potential for different ω_z: $\omega_z = 10$ (left) and $\omega_z = 1$ (right). The assignment of wave functions has been made by counting the number of nodal lines along the symmetric and antisymmetric electron coordinates for $\omega_z = 10$ (see text)

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