Spatial entanglement between electrons confined to rings

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We study systems of two and three electrons confined to circular rings. The electrons are considered spinless and we assume that one electron occupies a single ring. We use the framework of such a model to calculate the linear entropy and, thus, the spatial entanglement between the confined electrons. The geometry of the problem for the case of two electrons incorporates situations in which the planes of the two rings form an arbitrary angle with each other. The resulting Schrödinger's equation is solved numerically with very high accuracy by means of the exact diagonalization method. We compute the ground state energy and entanglement for all configurations under consideration. We also study the case of three electrons confined to identical, parallel and concentric rings which are located in three different equidistant planes. The vertically separated system of rings is allowed to gradually merge into a single ring geometry which would represent the equivalent system of a ring with three electrons. It is observed that the system of three electrons gives rise to a richer structure as the three rings merge into a single one.

Keywords: Spatial entanglement, Semiconductor heterojunction, Quantum dot, Quantum ring, Coulomb interaction

I. INTRODUCTION

Understanding correlation effects continues to be one of the most central problems in theoretical quantum chemistry and condensed matter physics. As a matter of fact, this has been the main goal of the majority of theories and models introduced in this research area [1, 2]. In particular, the behavior of electrons in low dimensions such as the two-dimensional (2D) electron gas [3] or 2D semiconductor systems [4–8] has been intensively studied during the past years. The interplay between confinement, quantum spin, delocalization effects and Coulomb repulsion between electrons under the dictate of quantum rules leads to many interesting physical phenomena and unanticipated patterns [9–11]. A system where considerable effort has been devoted in the past decade is the study of GaAs/AlGaAs concentric double quantum rings [12–16]. A double quantum ring system can be used to study the electronic transport and optical properties of various semiconducting materials [12–16]. For instance, the electronic transport in the system can be studied and controlled by means of external metallic electrodes that can be attached. Similarly, one can manipulate the electronic and optical properties of a double quantum ring by applying a laser field. By tuning the laser field one can create new degenerate energy levels and, thus, affect the optical properties of the system. Overall, a double quantum ring system has many possible technological applications with research topics ranging from opto-electronic properties to spin transport and/or quantum computation. The fabrication of such quantum rings was made possible by the invention of precise droplet-epitaxial techniques [17]. These nanosystems are extremely useful in order to gauge subtle quantum phenomena such as the Aharonov-Bohm effect [18] and the influence of the Coulomb interaction on the magnetic properties of small quantum systems of electrons [19].

In this study, we consider a concise model consisting of

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a few interacting electrons confined in distinct rings [20]. Each electron is allowed to occupy a single ring. For simplicity, the electrons are considered spinless. We, initially, consider a system of two electrons. The relative position of planes of the rings is allowed to change. This means that we are able to tune the geometry of the two rings in order to explore all relevant physical situations that involve the correlations between the two electrons. In addition to the model for two electrons, we also study another model of three electrons where each of them is confined to identical parallel coaxial rings situated in different equidistant planes. The three rings are allowed to merge forming a single ring as the inter-plane separation distance between them becomes zero. This special situation is tantamount to representing a system of three electrons confined to a single ring as far as the ground state and entanglement properties are concerned.

The present model of rings can be viewed as a simple presentation for more realistic realizations of double [21–23] or triple quantum ring systems [24, 25]. Double quantum rings typically consist of two concentric rings where the localization of electrons in each ring is provided by some confining potential. The confinement in both radial and azimuthal directions gives rise to interesting phenomena. The simplest approximation made would be to assume no radial extension with the electrons confined in an ideal ring where only the azimuthal angle varies. The aim of out model is to describe the entanglement effects between electrons separated in space in different rings. Therefore, it is a reasonable starting point to assume one electron per ring. This way we can pursue a theoretical investigation of the entanglement effects between electrons in different rings rather than having them in different states of the same ring. The model that we consider is simpler than typical experimental realization, but yet it is realistic enough to capture key features pertaining to entanglements effects in these structures. This work presents a study of a system of a few spinless electrons confined to circular rings with the assumption that one electron occupies a single ring. We calculate the linear entropy for ultra-small system of two or three electrons connected to distinct rings with an arbitrary geometry. The main goal is to estimate the amount of spatial entanglement between the electrons for the model under consideration as a function of the geometry parameters of the system.

The present contribution is organized as follows. In Section II we introduce the model for two and three electron systems, respectively. In Section III we describe the theoretical formalism and the numerical method used to calculate the entanglement between the electrons. The results for systems with two and three electrons are discussed in Section IV. Some brief conclusions are drawn in Section V.

II. MODEL

A. Two electrons

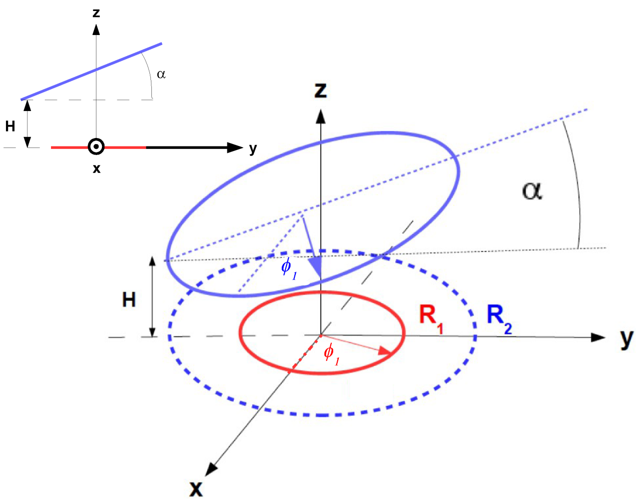

FIG. 1. (Color online) Relative position and geometry of two rings with radii, R_1 and R_2. Each of the rings contains one electron. The planes of the rings may be tilted relative to each other by an angle, α. Furthermore, the geometry of the system may range from coplanar to vertically separated (and tilted) double rings. A lateral view is also shown for clarification purposes. See text for details.

The model for two electrons and the geometry of the problem is illustrated by Fig. 1. We consider two different rings with respective radii, R_1 and R_2. We assume that $R_1 \leq R_2$. Electron 1 is located on the ring of radius, R_1 and electron 2 is located on the other ring of radius, R_2. Their location in these respective rings is determined by the azimuthal angles, ϕ_1 and ϕ_2. There can be a vertical distance, H separating the planar rings. Furthermore, the plane of ring 2 with radius, R_2 can be tilted by an angle α with respect to the $x-y$ plane of ring 1 at a minimum distance H from it. The two rings are parallel at a separation distance, H when the value of the tilting angle becomes zero ($\alpha = 0$). If this instance($\alpha = 0$ is projected on the $x - y$ plane, we have the dotted circumference with radius, R_2. A point of contact will appear at the position $(x = 0, y = -R, z = 0)$ if one reduces parameter H by keeping a nonzero tilting angle ($\alpha \neq 0$) and makes $R_1 = R_2 = R$. An additional inset in Fig. 1 displays the possibility of one ring being tilted with respect to the other. The electrons interact via the standard Coulomb interaction potential. The quantum Hamiltonian for the system of two electrons is written as:

$$\hat{H}(\phi_1, \phi_2) = -\frac{\hbar^2}{2\, m_e R_1^2} \frac{\partial^2}{\partial \phi_1^2} - \frac{\hbar^2}{2\, m_e R_2^2} \frac{\partial^2}{\partial \phi_2^2} + \frac{k\, e^2}{d(\phi_1, \phi_2)} \,, \tag{1}$$

where $\hbar$ is the reduced Planck's constant, m_e is the mass of the electrons, k is Coulomb's electric constant, e is the charge of the electron and $d(\phi_1,\phi_2) \equiv d(\phi_1,\phi_2;R_1,R_2,\alpha,H)$ is the separation distance between the pair of electrons. The square of such distance is given by:

$$\begin{aligned} d^2(\phi_1,\phi_2;R_1,R_2,\alpha,H) = & [R_2\cos\phi_2 - R_1\cos\phi_1]^2 + \\ & [R_2\cos\alpha - R_2 + R_2\cos\alpha\sin\phi_2 \\ & -R_1\sin\phi_1]^2 + \\ & [R_2\sin\alpha(1+\sin\phi_2)+H]^2 \ . \end{aligned} \tag{2}$$

No other subtler effects coming from electron's effective mass in a semiconductor host and/or from presence of a magnetic field are taken into account [26, 27].

The scenario with added tilting allows one to tune the quantum properties of the system of electrons by incorporating drastically different limiting cases that range from coplanar concentric double rings to vertically separated double rings with an arbitrary tilting. Therefore, the mere change of the geometric parameters may lead to fundamentally different quantum behavior of the system in a controllable fashion. Any effort in simplifying the quantity in Eq.(2) will not lead to a useful expression for our endeavor. Therefore, our main objective becomes the numerical solution of the resulting stationary Schrödinger's equation. Atomic units are used in which distances are measured in units of the Bohr radius, a_B while the energy is measured in the atomic unit of $k\,e^2/a_B$ (a Hartree), which is a commonly used in quantum atomic physics. At a formal level, one simply sets $\hbar = m_e = k = e = 1$. For this choice of units, the stationary Schrödinger's equation reads:

$$\begin{aligned} & -\frac{1}{2R_1^2}\frac{\partial^2}{\partial\phi_1^2}\Psi(\phi_1,\phi_2) - \frac{1}{2R_2^2}\frac{\partial^2}{\partial\phi_2^2}\Psi(\phi_1,\phi_2) \\ & +\frac{1}{d(\phi_1,\phi_2)}\Psi(\phi_1,\phi_2) \ = \ E\,\Psi(\phi_1,\phi_2) \ , \end{aligned} \tag{3}$$

where $\Psi(\phi_1,\phi_2)$ is the wave function for the system of two electrons, E is the energy eigenvalue and $0 \leq \phi_i < 0$ for $i = 1$ and 2. Note that the wave function for non-interacting particles is that of a particle confined in a circular ring with infinite potential wells outside the ring. The solution of the quantum problem is obviously periodic, $\Psi(0,\phi_2) = \Psi(2\pi,\phi_2)$ and $\Psi(\phi_1,0) = \Psi(\phi_1,2\pi)$. We use the following normalization condition:

$$R_1\,R_2\int_0^{2\,\pi}\int_0^{2\,\pi} d\phi_1\,d\phi_2\,|\Psi(\phi_1,\phi_2)|^2 \ = \ 1 \ . \tag{4}$$

The case $\alpha = 0$ is quasi-exactly solvable by using the distance between particles as a new variable. Although this analytic approach does not apply here, we can use such results to gauge the accuracy of our numerical computations.

B. Three electrons

The model of three electrons is a variation of the geometry of Fig. 1. For the setup of three electrons, we will have three vertically separated, parallel and concentric rings with the same radius, $R_1 = R_2 = R_3 = R = 1$ situated on three different equidistant parallel planes. Each ring will contain one single electron. For example, one ring is situated below the $x-y$ plane by a vertical distance, H (ring 1), a second ring is above such plane at a distance, H (ring 2) while the third ring is on the $x-y$ plane (ring 3). We believe that the reader can easily visualize the geometry of such a ring setup without need to draw a schematic presentation. The quantum Hamiltonian for the system of three electrons can be easily generalized from Eq.(1). The extension of the stationary Schrödinger's equation for such a case is straightforward (in atomic units):

$$\begin{aligned} & \sum_{i=1}^{3} -\frac{1}{2\,R^2}\frac{\partial^2}{\partial\phi_i^2}\Psi(\phi_1,\phi_2,\phi_3) \\ & +\frac{1}{d(\phi_1,\phi_2)}\Psi(\phi_1,\phi_2,\phi_3) \\ & +\frac{1}{d(\phi_1,\phi_3)}\Psi(\phi_1,\phi_2,\phi_3) \\ & +\frac{1}{d(\phi_2,\phi_3)}\Psi(\phi_1,\phi_2,\phi_3) \ = \ E\,\Psi(\phi_1,\phi_2,\phi_3) \ , \end{aligned} \tag{5}$$

where $\Psi(\phi_1,\phi_2,\phi_3)$ is the wave function for three electrons, E is the corresponding energy eigenvalue of the system and, in this scenario, $d(\phi_i,\phi_j) \equiv d(\phi_i,\phi_j;R,R,\alpha=0,H)$ are the separation distances between pairs of electrons written in short-hand notation. Obviously, the same periodicity properties are imposed on the wave function.

III. THEORY AND METHOD

A. Spatial entanglement

A natural question that emerges is what happens to the quantum system under consideration when the geometry of the Hamiltonian changes. One quantum information-based measure of the spatial entanglement (mixedness) in quantum states is the so-called linear entropy defined as:

$$\mathcal{E} = 1 \ - \ \mathrm{Tr}[\rho_r^2] \ , \tag{6}$$

where Tr is the trace operation and ρ_r is the single-particle reduced density matrix [28] of the state:

$$\rho_r = \int d\phi_2\,\Psi(\phi_1,\phi_2)\,\Psi^*(\phi_1{}',\phi_2) \ . \tag{7}$$

One can check that:

$$\begin{aligned} \mathrm{Tr}[\rho_r^2] = \int d\phi_1\,d\phi_1{}'\,d\phi_2\,d\phi_2{}'\,\Psi(\phi_1,\phi_2)\,\Psi^*(\phi_1{}',\phi_2) \\ \Psi^*(\phi_1,\phi_2{}')\,\Psi(\phi_1{}',\phi_2{}') \ . \end{aligned} \tag{8}$$

Note that the calculation of the linear entropy is a rather involved mathematical process. The linear entropy defined in Eq.(6) is quite popular for the analysis of entanglement in two-particle systems and has been pursued at length in the literature [29–34].

Our objective in this work is to obtain the entanglement measure, $\mathcal{E}$ defined in Eq.(6) for various combinations of the geometry of the system. To be more specific, we will consider the following four cases:

- $\alpha = 0$, $H = 0$ which reduces to the case of two coplanar concentric rings studied in [35]. The special case, $R_1 = R_2$ implies two electrons in the same ring.
- $\alpha = 0$ and $H \neq 0$ reduces to the case of two electrons in vertically coupled parallel rings studied in [36].
- $\alpha = 0$, $H = 0$ and $R_1 \approx R_2$ where both radii increase, but they differ slightly from each other.
- $\alpha \neq 0$ and $R_1 \approx R_2$ which corresponds to two rings that almost share a point of contact since α is tilted and $R_1 \neq R_2$ (since they differ slightly).

All these cases are studied numerically by solving the the stationary Schrödinger's equation via the exact diagonalization method.

B. Numerical method

Let us illustrate the exact numerical diagonalization approach for the system of two electrons. One easy way of preserving the periodicity of the solution is to span the (unknown) wave function, $\Psi(\phi_1, \phi_2)$ in the basis of the eigenstates for two non-interacting electrons each one in its respective ring and then truncate the expansion to $N+1$ terms where N even. That is:

$$\Psi(\phi_1,\phi_2) \;=\; \sum_{m=-\frac{N}{2}}^{\frac{N}{2}} \sum_{n=-\frac{N}{2}}^{\frac{N}{2}} c_{m,n}\, \frac{1}{2\pi\sqrt{R_1R_2}} e^{im\phi_1} e^{in\phi_2} \tag{9}$$

By substituting Eq.(9) into Eq.(3), multiplying by $\frac{1}{2\pi\sqrt{R_1R_2}} e^{-ik\phi_1} e^{-il\phi_2}$ and integrating over the angles, ϕ_1 and ϕ_2 we obtain:

$$\sum_{k=-\frac{N}{2}}^{\frac{N}{2}} \sum_{l=-\frac{N}{2}}^{\frac{N}{2}} \Bigg[\left(\frac{m^2}{2R_1^2} + \frac{n^2}{2R_2^2}\right)\delta_{k,m}\delta_{l,n} + \langle kl|\frac{1}{d}|mn\rangle \\ -E\,\delta_{k,m}\delta_{l,n}\Bigg] c_{k,l} \;=\; 0 \;, \tag{10}$$

for indices, $m,n = -\frac{N}{2},..,\frac{N}{2}$. Let us denote by H_{klmn} the first line in Eq.(10). Solving Eq.(10) for $c_{k,l}$ is tantamount to providing an approximate solution to Eq.(3) for both ground and excited states. One can increase the accuracy of the calculations by augmenting the number of terms in the expansion.

The Coulomb interaction matrix element shown in Eq.(10) reads explicitly as:

$$\langle kl|\frac{1}{d}|mn\rangle \;=\; \frac{1}{4\pi^2}\int_0^{2\pi}\int_0^{2\pi} d\phi_1 d\phi_2\, \frac{e^{i(m-k)\phi_1} e^{i(n-l)\phi_2}}{d(\phi_1,\phi_2)}. \tag{11}$$

The set of equations in Eq.(10) for $c_{k,l}$ does not read yet as a standard eigenvalue problem. In order to do so, one must transform $H_{klmn} \longrightarrow A_{ij}$ and $c_{k,l} \longrightarrow g_j$, $i,j = 1,..,(N+1)^2$ using $i = (m+\frac{N}{2})(N+1)+(n+\frac{N}{2})+1$ and $j = (k+\frac{N}{2})(N+1)+(l+\frac{N}{2})+1 \;\forall\,(k,l,m,n)$. With this transformation, we have the usual eigenvalue and eigenvector problem:

$$\sum_{j=1}^{(N+1)^2} \left(A_{ij} - E\,\delta_{ij}\right) g_j \;=\; 0 \;, \tag{12}$$

where $i = 1,2,..,(N+1)^2$. Finding the corresponding energy eigenvalues will give as the energy spectrum of the system. In order to find the eigenvectors, the inverse transformation $g_j \longrightarrow c_{k,l}$ can be proved to be unique. In other words, given j and N, we find a sole couple (k,l).

Once the coefficients $c_{k,l}$ are obtained, it is straightforward to obtain the wave function and, thus, calculate the linear entropy as defined in Eq.(6). To this aim, we use the fact that the ultimate integration turns out to be on separate arguments provided that we use Eq.(9) together with the orthogonality condition. The value of linear entropy:

$$\mathcal{E} = 1 - \sum_{a=-\frac{N}{2}}^{\frac{N}{2}} \sum_{b=-\frac{N}{2}}^{\frac{N}{2}} \sum_{c=-\frac{N}{2}}^{\frac{N}{2}} \sum_{d=-\frac{N}{2}}^{\frac{N}{2}} c_{a,b}\, c^*_{c,b}\, c^*_{a,d}\, c_{c,d} \;, \tag{13}$$

is obtained numerically once the desired numerical accuracy is met.

C. Numerical validation

In order to validate the accuracy of the numerical results, we compare them to the analytic case of two electrons in concentric rings [35]. The results for the expansion coefficients of the ground state wave function are shown in Table. I. The matching is perfect.

The corresponding ground state wave function is shown in Fig. 2 where $\Psi(\phi_1,\phi_2)$ is plotted. Note that the wave function is expressed as a linear combination of terms for negative, zero and positive indices. It happens that the expansion coefficients, $c_{k,l}$ have the same value for opposite indices. Therefore, the outcome is a purely real ground state wave function meaning that $\Psi(\phi_1,\phi_2) = |\Psi(\phi_1,\phi_2)|$ where the latter would represent the (real) modulus of the wave function. It is worth mentioning that, as in Table. I, it will be enough to have a

k	l	$c_{k,l}$
-5	5	4.52937008×10^{-5}
-4	4	0.000210684568
-3	3	0.00133573123
-2	2	0.0393656555
-1	1	-0.401700424
0	0	0.821078904
1	-1	-0.401700424
2	-2	0.0393656555
3	-3	0.00133573123
4	-4	0.000210684568
5	-5	4.52937008×10^{-5}

TABLE I. Expansion coefficients, $c_{k,l}$ corresponding to the ground state wave function solution for the analytic case, $R_1 = \frac{13}{7}\sqrt{3(13-\sqrt{78})}$, $R_2 = \frac{13}{7}\sqrt{3(13+\sqrt{78})}$, $H = 0$ and $\alpha = 0$. The ground state energy that we calculated numerically is virtually equal to the exact value of $\frac{28}{507}$. The linear entropy was found to be 0.493413059. Notice the symmetry in the indexes k, l and in the numerical value of $c_{k,l}$. As one can notice, the numerical solution is accurately obtained with only 11 expansion coefficients, $c_{k,l}$. See text for details.

basis set with $N = 10$ for the linear expansion in Eq.(9) for all cases considered. The case of two electrons in vertically coupled rings has also quasi-exact analytic solutions [36]. The corresponding results for the expansion coefficients of the ground state wave function are displayed in Table. II.

k	l	$c_{k,l}$
-5	5	4.52937079×10^{-5}
-4	4	0.00021068459
-3	3	0.00133573128
-2	2	0.0393656611
-1	1	-0.401700435
0	0	0.821078894
1	-1	-0.401700435
2	-2	0.0393656611
3	-3	0.00133573128
4	-4	0.00021068459
5	-5	4.52937079×10^{-5}

TABLE II. Solution coefficients $c_{k,l}$ for the analytic case $R_1 = R_2 = R = \frac{13^{3/4}\sqrt{3}}{7^{1/4}}$, $H = R\frac{\sqrt{2}\sqrt{\sqrt{13}-\sqrt{7}}}{7^{1/4}}$ and $\alpha = 0$. The numerically calculated ground state energy is virtually equal to the analytic value, $\frac{4\sqrt{7/13}}{39}$. The linear entropy is found to be 0.493413077. Notice the astonishing similarity between the values of the expansion coefficients for the present case and their concentric counterparts shown in Table I. Totally different geometric configurations result in almost the same solution coefficients, $c_{k,l}$ and, consequently, the same linear entropy value. See text for details.

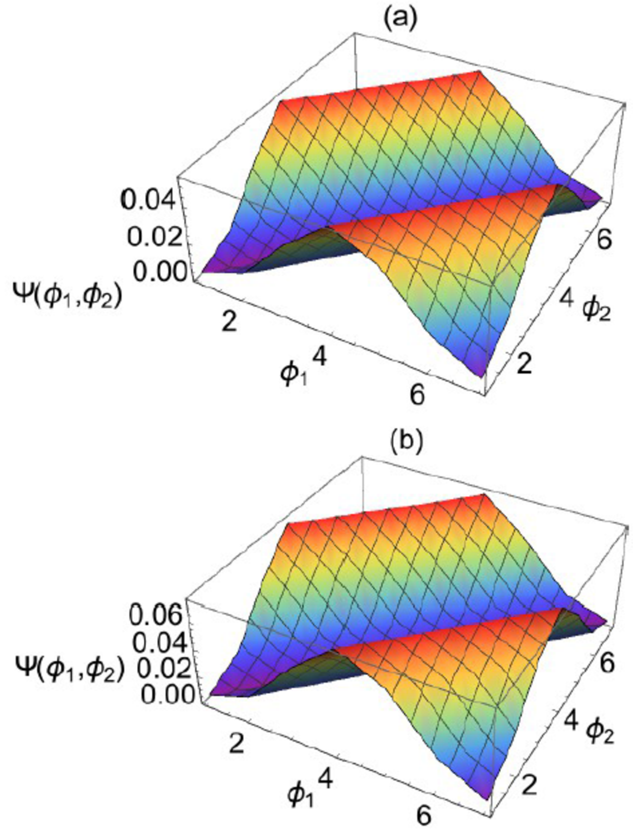

FIG. 2. (Color online) (a) Plot for the ground state wave function for $R_1 = \frac{13}{7}\sqrt{3(13-\sqrt{78})}$, $R_2 = \frac{13}{7}\sqrt{3(13+\sqrt{78})}$, $H = 0$ and $\alpha = 0$. (b) Similar plot for $R_1 = R_2 = R = \frac{13^{3/4}\sqrt{3}}{7^{1/4}}$, $H = R\frac{\sqrt{2}\sqrt{\sqrt{13}-\sqrt{7}}}{7^{1/4}}$ and $\alpha = 0$. The two plots look very similar because the obtained corresponding coefficients, $c_{k,l}$ have very small differences. See text for details.

It is indeed remarkable to see that the expansion coefficients, $c_{k,l}$ are almost identical in both cases. Having different geometries, we cannot explain why the two instances, although returning different ground state energies, provide the same answer as far as the wave function and entanglement are concerned. In both cases, concomitant wave functions have very low values when $\phi_1 = \phi_2$ due to the strong Coulomb repulsion.

In any case, the symmetry of the coefficients has a twofold meaning. On one hand, the total truncated state is real, whereas on the other hand, the system depends only on the difference of angles, $|\phi_1 - \phi_2|$. The method of spanning the function in a suitable basis is quite convenient. Although the treatment is numerical, the final result represents accurately the exact eigenvalue when the number of elements in the expansion basis tends to infinity. For our system of two electrons in two coplanar concentric rings, the 11 expansion coefficients for the ground state wave function are available from Table I. By analyzing the 121×121 matrix elements of A_{ij}, one can observe typical parabolas as a function of the indices i, j corresponding to free electrons in a ring. What is remarkable is that almost all the matrix elements intervene in determining the value of the ground state energy, E_0. In other words, there is no such subset that makes it easier to diagonalize the matrix, A_{ij} and thus find, E_0. This seems to be the most likely scenario in all cases.

The extension of the calculations to three electrons is straightforward, though it becomes computationally more demanding. The wave function $\Psi(\phi_1, \phi_2, \phi_3)$ reads (all radii are equal):

$$\sum_{n_1=-\frac{N}{2}}^{\frac{N}{2}} \sum_{n_2=-\frac{N}{2}}^{\frac{N}{2}} \sum_{n_3=-\frac{N}{2}}^{\frac{N}{2}} c_{n_1,n_2,n_3} \frac{1}{\sqrt{2\pi R}^3} e^{i(n_1\phi_1+n_2\phi_2+n_3\phi_3)} . \tag{14}$$

Proceeding as before, the set of equations to solve is:

$$\begin{aligned}\sum_{k_1=-\frac{N}{2}}^{\frac{N}{2}} \sum_{k_2=-\frac{N}{2}}^{\frac{N}{2}} \sum_{k_3=-\frac{N}{2}}^{\frac{N}{2}} \Bigg[\left(\frac{n_1^2}{2R^2} + \frac{n_2^2}{2R^2} + \frac{n_3^2}{2R^2} \right) \delta_{\{k_i,n_i\}} \\ + \langle k_1 k_2 | \frac{1}{d(\phi_1,\phi_2)} | n_1 n_2 \rangle \delta_{k_3,n_3} \\ + \langle k_1 k_3 | \frac{1}{d(\phi_1,\phi_3)} | n_1 n_3 \rangle \delta_{k_2,n_2} \\ + \langle k_2 k_3 | \frac{1}{d(\phi_2,\phi_3)} | n_2 n_3 \rangle \delta_{k_1,n_1} \\ - E\,\delta_{\{k_i,n_i\}} \Bigg] c_{k_1,k_2,k_3} = 0 \ , \end{aligned} \tag{15}$$

with $\delta_{\{k_i,n_i\}} \equiv \delta_{k_1,n_1}\delta_{k_2,n_2}\delta_{k_3,n_3}$ and $n_1, n_2, n_3 = -\frac{N}{2}, .., \frac{N}{2}$. The addition of a new electron makes the whole computation grow from a $(N+1)^2 \times (N+1)^2$ matrix to $(N+1)^3 \times (N+1)^3$ (recall that N is an even number). This is so because in order to accommodate an additional index into a square matrix, we have to perform the transformation $i = (n_1 + \frac{N}{2})(N+1)^2 + (n_2 + \frac{N}{2})(N+1) + (n_3 + \frac{N}{2}) + 1$ and $j = (k_1 + \frac{N}{2})(N+1)^2 + (k_2 + \frac{N}{2})(N+1) + (k_3 + \frac{N}{2}) + 1 \ \forall\, (k_1 k_2, k_3, n_1, n_2, n_3)$. With this transformation, we then have the usual eigenvalue and eigenvector problem:

$$\sum_{j=1}^{(N+1)^3} \left(A_{ij} - E\,\delta_{ij} \right) g_j = 0 \ , \tag{16}$$

where $i = 1, 2, .., (N+1)^3$. In practice, we shall use a value of $N = 8$ which implies a total of 9 basis elements for the system of three electrons. For the case of the computation of entanglement between pairs, the expression in Eq.(13) remains the same provided we make zero the subindex in $c_{a,b,c}$ belonging to the particle not involved.

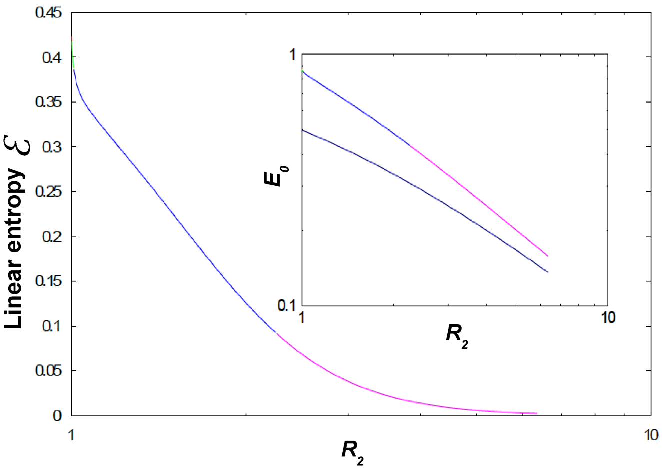

FIG. 3. (Color online) Plot of the linear entropy (entanglement), $\mathcal{E}$ between the two electrons when the corresponding rings are coplanar and concentric with $R_1 = 1$ and R_2 that increases its value. In this semi-logarithmic plot (with the axis of R_2 shown in a logarithmic scale), we can identify a region where an exponential decay takes place. The inset depicts the ground state energy, E_0 as a function of R_2 alongside with the classical result (lower curve). See text for details.

IV. RESULTS

A. Two rings

Before discussing each configuration separately, we like to draw attention to the fact that the classical equilibrium energy for the system of two electrons in separate planar concentric rings is $\frac{1}{R_1+R_2}$. We remind the reader that the energy values are given in atomic units. It is notable that this value is close to the quantum ground state energy value, E_0. Thus, for those instances where we have coplanar rings, we will compare the quantum ground state energy, E_0 with its classical counterpart.

1. *Two coplanar concentric rings ($R_1 \neq R_2$)*

We consider two coplanar concentric rings ($H = 0$ and $\alpha = 0$). We set $R_1 = 1$ while R_2 is treated as a variable with the condition that $R_2 > R_1$. The linear entropy (entanglement), $\mathcal{E}$ and the ground state energy, E_0 are depicted in Fig. 3. The lower curve in the inset represents the classical equilibrium energy.

2. *Two almost identical vertically separated parallel coaxial rings ($R_1 \approx R_2$)*

We consider two vertically separated parallel coaxial rings ($H \neq 0$ and $\alpha = 0$). We assume that the rings are almost identical by setting the values of their respective radii to $R_1 = 1$ and $R_2 = 1.01$. The variable for the present case is the vertical separation distance, H between the rings. The linear entropy, $\mathcal{E}$ and ground state energy, E_0 are shown in Fig. 4 as a function of H.

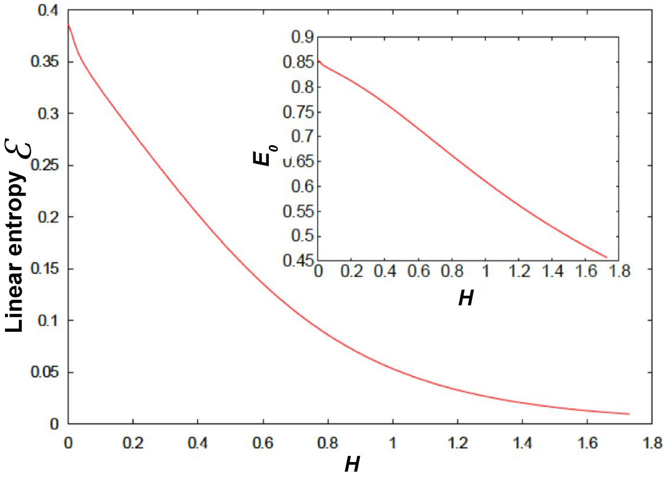

FIG. 4. (Color online) Plot of the linear entropy (entanglement), $\mathcal{E}$ between the two electrons and ground state energy of the system, E_0 as a function of the vertical separation distance, H between the two rings. The value of H changes from 0 to a maximum of 1.8. See text for details.

3. *Two almost identical coplanar concentric rings ($R_1 \approx R_2$)*

Here we consider two coplanar concentric rings ($H = 0$ and $\alpha = 0$) that are almost identical to each other. For such a case, we assume $R_1 = R$, $R_2 = R + 0.01$ with R being treated as a variable. The linear entropy and the ground state energy as a function of R are depicted in Fig. 5. In all other cases, both ground state energy and entanglement decreases. However, in the present instance, entanglement increases as R increases. The ground state energy of the system, E_0 is followed closely from below by its classical equilibrium counterpart (lower curve in the inset of Fig. 5). Note an almost power-law decay of E_0 as a function of R which is not present in the previous scenarios.

4. *Two almost identical tilted rings forming an angle α ($R_1 \approx R_2$)*

The last possible situation that we studied is that of two almost identical rings with respective radii, $R_1 = 1$ and $R_2 = 1.01$ which are tilted by a given angle relative to each other. For such a situation, we consider $R_1 = 1$, $R_2 = 1.01$ and $H = 0$ and tilt the second ring, R_2 by some angle, α as shown in Fig. 1. The corresponding results for the ground state energy, E_0 and linear entropy, $\mathcal{E}$ as a function of angle, α are depicted in Fig. 6. As expected, two coplanar rings that are tangent to each other ($\alpha = 0$) have much less entanglement than for any other angle.

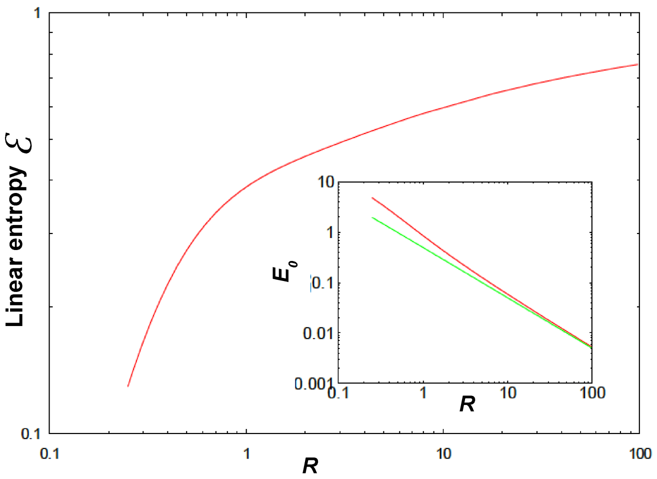

FIG. 5. (Color online) Plot of the linear entropy (entanglement), $\mathcal{E}$ as a function of R for two electrons in coplanar concentric rings with radii that grow in such a way that $R_1 = R$, $R_2 = R + 0.01$ under the constraint, $R_2 - R_1 = 0.01$. In this case, R is the variable. This constraint is imposed in order to have two rings with almost the same radius. The axis of R is shown in a logarithmic scale. It is the only instance considered where the entanglement between the electrons increases as the radius, $R_1 = R$ of the inner ring increases. Also, note in the inset how close the ground state energy, E_0 is to its classical counterpart (lower curve). See text for details.

B. Three rings

As we will see, the case of three electrons with each of them confined to one of the three vertically separated parallel rings manifests a much richer structure than the corresponding cases of two electrons. The ultimate scenario that we are interested to study is that of three rings merging into a single one while decreasing their separation distance, H. Larger systems are more demanding to be handled numerically. However, we note that a total of 9 basis sets will still suffice to calculate with enough precision the energy and entanglement of the system of three electrons. The energy of the ground state and the first, second and third excited state energies are plotted in Fig. 7 as a function of the distance between the planes, H. The first and second excited states are degenerate up to values of $H = 0.001$ where they have the same energy. Thus, we focus our attention on the ground state energy. It is apparent that at some point around the value $H = 0.004$ there is a level crossing of the energy as enhanced in the inset of Fig. 7. By employing the cur-

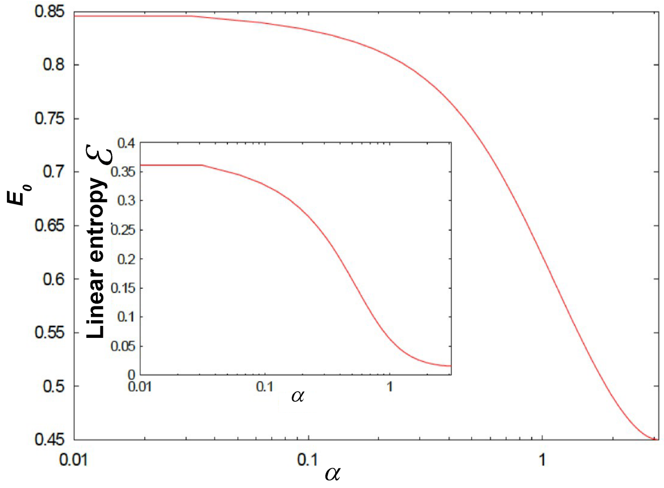

FIG. 6. (Color online) Ground state energy, E_0 and linear entropy (entanglement), $\mathcal{E}$ as a function of tilting angle, α ranging from 0 to π shown as a semi-logarithmic plot (with the axis of α shown in a logarithmic scale). This geometric configuration has not been considered previously in the literature. See text for details.

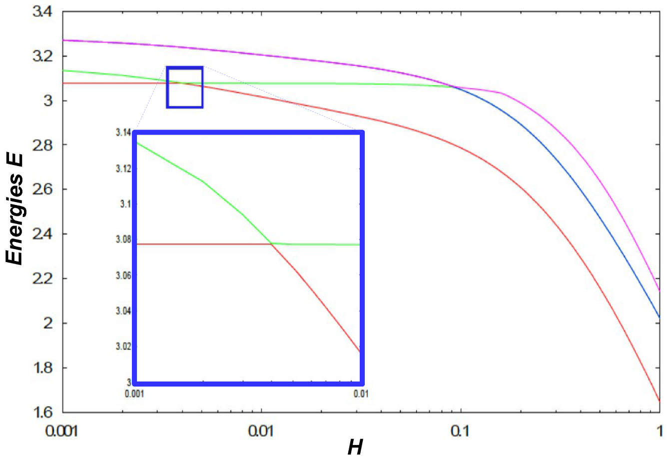

FIG. 7. (Color online) Plot of the first three eigen-energies, E for the system of three electrons as function of the distance between planes, H. The axis of H is shown in a logarithmic scale. The first and second excited states are degenerate, thus, have the same energy. There is a level-crossing at some point as H decreases (detailed in the inset). See text for details.

rent method, we can assess that the ground state energy is not greater than $E_0 = 3.0775$ (in atomic units) in the $H \to 0$ limit. However, it is only when we study the entanglement between the electrons in the rings that we can appreciate a change in the structure of the ground state. The two-party, namely, bipartite (or pairwise) entanglement in the system is depicted in Fig. 8. Due to symmetry reasons, nearest-neighbors rings have the same entanglement. Only the next-to-nearest neighbor case differs slightly. Actually, all the three pairs tend to the same value as H decreases.

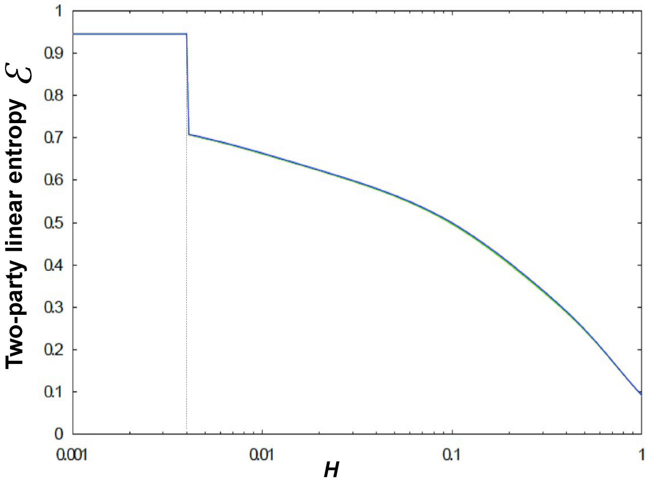

FIG. 8. (Color online) Plot of the three pairwise entanglement quantities as the distance between planes H for the three-particle case diminishes. The axis of H is shown in a logarithmic scale. A discontinuous jump is shown due to the level crossing in energy. Normally, a level crossing arises from a phase transition or symmetry breaking. The level-crossing in Fig. 7 indicates an abrupt change in the structure of the ground state very close to $H = 0$. This would be the only factor that can account for a different entanglement. See text for details.

This situation does not occur for the corresponding case of two electrons due to the nature of their energy spectrum. This intriguing fact is very interesting for two main reasons. First, we have to go to considerably small values of H to see this effect with the result collapsing to a constant value for smaller values of H. Does this imply that the three electrons system can now be regarded as an effective three particle system inside the same ring? Secondly, it is not easy to predict the implications that this very remarkable feature may have for other quantities besides entanglement and ground state energy. Therefore, it is of great interest to study if this phenomenon occurs for systems with a much larger number of electrons. Unfortunately, such a problem is very challenging to solve even from a numerical perspective.

In order to further assess the properties of the system of three particles in the extreme cases of $H = 1$ and $H = 0.001$ we have depicted two ways of visualizing the related ground state wave function, $\Psi(\phi_1, \phi_2, \phi_3)$. Note that the corresponding numerical values of the expansion coefficients for the ground state wave function are given in the Appendix.

The first way belongs to Fig. 9 where the magnitude square of the ground state wave function, $|\Psi(\phi_1, \phi_2, \phi_3)|^2$ is plotted as a function of angle differences, $\phi_2 - \phi_1$ and

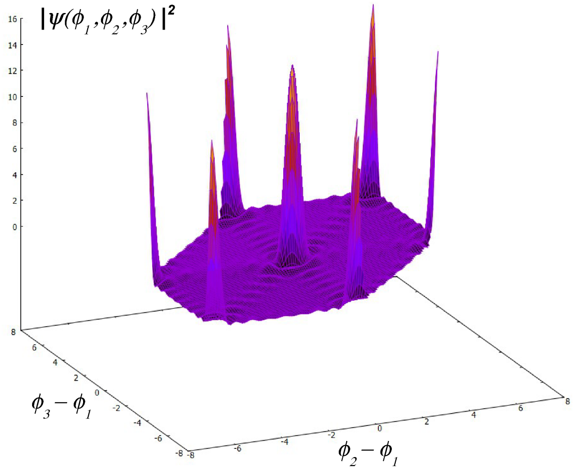

FIG. 9. (Color online) Plot of $|\Psi(\phi_1,\phi_2,\phi_3)|^2$ (ground state) as a function of angle differences, $\phi_2-\phi_1$ and $\phi_3-\phi_1$ for a value of $H=1$. Notice the central high peak value. In the light of this result, it can be argued that the three electrons have the largest overlap for nearly the same angular position. See text for details.

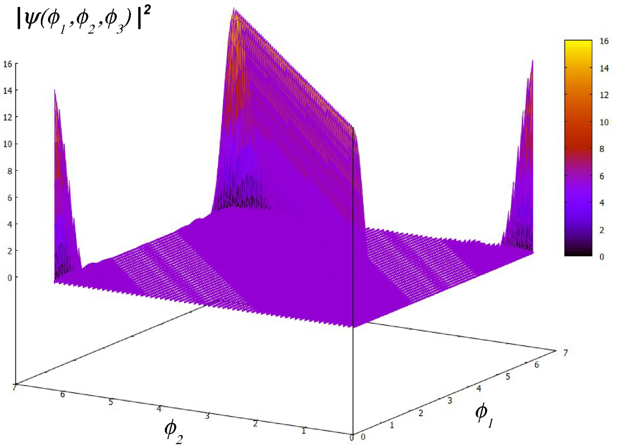

FIG. 10. (Color online) Plot of $|\Psi(\phi_1,\phi_2,\phi_3)|^2$ (ground state) as a function of the angles, ϕ_1 and ϕ_2 of the electrons in the two neighboring rings and $H=1$. Note that the third angle ϕ_3 runs free and takes all the possible values from 0 to 2π. A similar situation for small H (not shown) does not change much the overall result. The high probability of finding any two electrons being close is apparent. See text for details.

$\phi_3-\phi_1$ for a value of $H=1$. One can appreciate the fact that electrons tend to be localized around the same position.

The second way is illustrated by Fig. 10 where we show $|\Psi(\phi_1,\phi_2,\phi_3)|^2$ as a function of angles, ϕ_1 and ϕ_2 for a value of $H=1$. It is plainly clear to argue that, most likely, one can find the electrons localized in the same region. Also, the probability density is zero when the value of the angles are far apart. A similar behavior occurs for $H=0.001$ (not displayed). This is the situation pertaining to three electrons being practically located in the same ring. The main difference with respect to the $H=1$ case is that the previous regions of zero probability are now filled with non-negligible "bumps" which account for a different structure in the ground state of the system.

V. CONCLUSIONS

In conclusion, this work deals with some ultra-small systems consisting of two or three electrons. The electrons are confined to move in circular rings. It is assumed that the electrons are spinless and that each ring is occupied by a single electron. We consider various geometries for the setup of rings and this makes this problem rather challenging. The resulting general quantum problem cannot be solved exactly in analytical form. Therefore, in order to obtain the energy and wave function for the systems under consideration we resort to the use of the exact numerical diagonalization method. We use such a framework to calculate the linear entropy for two and three electron systems while allowing the geometry of the problem to change between various scenarios. The exact numerical diagonalization method that we use can be extended to systems with more than three electrons. However, the computational costs and the time to complete the calculations grows very fast as the number of electrons grows. For this reason we limited our calculations to systems with only two and three electrons in order to carry out accurate calculations within a reasonable amount of computer time.

To this effect we implemented accurate exact numerical diagonalization calculations by using an exact basis truncation method in order to solve the quantum problem. This approach allows us to obtain the energies, linear entropy and entanglement between the two electrons in the two rings for rings that have different possible geometric configurations. The ground state energy and entanglement is numerically calculated for all the configurations considered. By using the same procedure, we studied also the model of three electrons each occupying vertically separated identical coaxial rings. The special situation of three electrons with the three rings being merged into a single one is also analyzed. We find some surprising results as far as the localization of the particles is concerned for such a case. We also observe an interesting discontinuous increase in the entanglement between pairs as the distance between the rings tends to zero.

AUTHOR CONTRIBUTIONS

Conceptualization, O.C. and J.B.; Methodology, O.C., J.B., M.A.-A., M.A.H. and S.A.; Software, J.B.; Validation, O.C., J.B., M.A.-A., M.A.H. and S.A.; Formal analysis, O.C. and J.B.; Data curation, J.B.; Writing—review & editing, O.C. and J.B. All authors have read and agreed to the published version of the manuscript.

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DATA AVAILABILITY STATEMENT

The data presented in this study are available upon request from the authors.

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CONFLICTS OF INTEREST

The authors declare no conflicts of interest. The funders had no role in the design of the study; in the collection, analyses, or interpretation of data; in the writing of the manuscript; or in the decision to publish the results.

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APPENDIX

In this Appendix we present the explicit values of the expansion coefficients for the ground state wave function of three electrons. The values of c_{k_1,k_2,k_3} for $R_1 = R_2 = R_3 = 1$ and $H = 1$ are shown in Table. III. Those for $H = 0.001$ are shown in Table. IV.

k_1	k_2	k_3	c_{k_1,k_2,k_3}
-4	0	4	-0.000131476609
-4	1	3	7.41767774×10^{-5}
-4	2	2	1.53017668×10^{-5}
-4	3	1	7.41767774×10^{-5}
-4	4	0	-0.000131476609
-3	-1	4	3.09465428×10^{-5}
-3	0	3	-0.000698293354
-3	1	2	0.000480345404
-3	2	1	0.000480345404
-3	3	0	-0.000698293354
-3	4	-1	3.09465428×10^{-5}
-2	-2	4	2.12479165×10^{-6}
-2	-1	3	0.000190306552
-2	0	2	-0.00520647438
-2	1	1	0.00909765478
-2	2	0	-0.00520647438
-2	3	-1	0.000190306552
-2	4	-2	2.12479165×10^{-6}
-1	-3	4	5.40595983×10^{-6}
-1	-2	3	7.70769349×10^{-5}
-1	-1	2	0.00328129173
-1	0	1	-0.107830758
-1	1	0	-0.107830758
-1	2	-1	0.00328129173
-1	3	-2	7.70769349×10^{-5}
-1	4	-3	5.40595983×10^{-6}
0	-4	4	-5.26775736×10^{-6}
0	-3	3	-6.4193788×10^{-5}
0	-2	2	-0.0011496827
0	-1	1	-0.00899787456
0	0	0	0.976219937

TABLE III. Expansion coefficients, c_{k_1,k_2,k_3} for the ground state wave function solution for the system of three electrons when $R_1 = R_2 = R_3 = 1$ and $H = 1$. The rest of the coefficients not shown are obtained by changing the sign of the set of integers $\{k_i\}$. They are exactly equal to the c_{k_1,k_2,k_3} shown here. We have used a basis set with $N = 8$.

k_1	k_2	k_3	c_{k_1,k_2,k_3}
-4	0	4	-0.00300389246
-4	1	3	0.00264379189
-4	3	1	-0.00264379189
-4	4	0	0.00300389246
-3	-1	4	0.00264382094
-3	0	3	-0.00815690883
-3	1	2	0.00950729392
-3	2	1	-0.00950729392
-3	3	0	0.00815690883
-3	4	-1	-0.00264382094
-2	-1	3	0.00950731754
-2	0	2	-0.0377186212
-2	2	0	0.0377186212
-2	3	-1	-0.00950731754
-1	-3	4	-0.00264370077
-1	-2	3	-0.00950718227
-1	0	1	0.406169353
-1	1	0	-0.406169353
-1	3	-2	0.00950718227
-1	4	-3	0.00264370077
0	-4	4	0.00300376913
0	-3	3	0.0081566846
0	-2	2	0.0377181052
0	-1	1	-0.406169831

TABLE IV. Expansion coefficients, c_{k_1,k_2,k_3} for the ground state wave function solution for the system of three electrons when $R_1 = R_2 = R_3 = 1$ and $H = 0.001$. This is the scenario for which the three electrons are practically located in the same ring. The rest of the coefficients not shown are obtained by changing the sign of the set of integers $\{k_i\}$ and are exactly the opposite of the c_{k_1,k_2,k_3} coefficients shown here. Notice the change of structure with respect to the $H = 1$ case. We have used a basis set with $N = 8$.