Exact wave functions of two-electron quantum rings

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We demonstrate that the Schrödinger equation for two electrons on a ring, which is the usual paradigm to model quantum rings, is solvable in closed form for particular values of the radius. We show that both polynomial and irrational solutions can be found for any value of the angular momentum and that the singlet and triplet manifolds, which are degenerate, have distinct geometric phases. We also study the nodal structure associated with these two-electron states.

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Introduction.—Like quantum dots [1], quantum rings (QR) are self-organized nanometric semiconductors, and are intensively studied experimentally due to their rich electronic, magnetic and optical properties [2–7], such as the Aharonov-Bohm effect [8–10].

Many-electron QRs have been investigated theoretically using various methods, such as model Hamiltonian [11–13], exact diagonalization [14–15], quantum Monte Carlo [15–16], and density-functional theory [17–20] (DFT). Accurate numerical calculations on two-electron QRs have been reported in Ref. [21].

Quantum rings are usually modelled by electrons confined to a strict- or quasi-one-dimensional circular space interacting via a short-ranged or Coulomb operator. In this Letter, we focus on the simple system in which two electrons are confined to a ring of radius \( R \) and interact via a Coulomb operator. This choice has often been avoided in the literature due to the divergence of the Coulomb interaction at small interelectronic distances.

Contrary to frequent claims, systems with two electrons do not inevitably have intractable Schrödinger equations and we show here that, for each electronic state of a two-electron QR, the Schrodinger equation can be solved exactly for a countably infinite set of \( R \) values, yielding both polynomial and irrational solutions in terms of the interelectronic distance. Quantum mechanical systems whose Schrödinger equations can be solved in this way, such as the Hooke’s law [22] or spherium [23, 24] atoms, have ongoing value both for illuminating more complicated systems [25–26] and for testing and developing theoretical approaches, such as DFT [27,30] and explicitly correlated methods [31].

In atomic units (\( \hbar = m = e = 1 \)), the Hamiltonian of two electrons on a ring of radius \( R \) is

\[
\hat{H} = \frac{1}{2} (p_1^2 + p_2^2) + \frac{1}{u},
\]

(1)

where \( p_k = (i/R)\partial/\partial\theta_k \) is the momentum operator associated with the electron \( k \), and \( \theta_k \) is its angle around the ring center. The operator \( u^{-1} \) represents the Coulomb interaction between the electrons, where

\[
u = R\sqrt{2 - 2\cos(\theta_1 - \theta_2)}
\]

(2)
is the interelectronic distance [32]. In one dimension, the singlet and triplet manifolds are degenerate [33] and this allows us to focus primarily on the singlets.

Hartree-Fock solution.—Within the Hartree-Fock approximation [34], the ground-state wave function is simply

\[
\Psi_{HF}(\mathbf{u}) = u,
\]

(3)

which has a node at \( u = 0 \), and the energy is

\[
\epsilon_{HF} = \frac{1}{4R^2} + \frac{2}{\pi R}.
\]

(4)

Exact solution.—In terms of the extracule coordinate \( \Omega = (\theta_1 + \theta_2)/2 \) and intracule coordinate \( \omega = \theta_1 - \theta_2 \) [35], the Hamiltonian (1) is \( \hat{H} = \hat{H}_\Omega + \hat{H}_\omega \), where

\[
\hat{H}_\Omega = -\frac{1}{4R^2} \frac{\partial^2}{\partial\Omega^2},
\]

(5)

\[
\hat{H}_\omega = -\frac{1}{R^2} \frac{\partial^2}{\partial\omega^2} + \frac{1}{R\sqrt{2 - 2\cos\omega}},
\]

(6)
The exact spatial wave function is then the product

\[
\Phi(\Omega, \omega) = \Lambda(\Omega)\Psi(\omega),
\]

(7)
and the exact total energy is the sum \( E = \mathcal{E} + \epsilon \) of the extraculare and intraculare energies.

The eigenfunctions and eigenvalues of \( \hat{H}_\Omega \) are

\[
\Lambda_J(\Omega) = \exp (iJ\Omega), \quad \mathcal{E}_J = \frac{J^2}{4R^2},
\]

(8)
where \( J \in \mathbb{N} \) is the total angular momentum associated with the center-of-mass coordinate [36].
The eigenfunctions of $H_{\omega}$ satisfy
\[
-\frac{\Psi''(\omega)}{R^2} + \frac{\Psi(\omega)}{R \sqrt{2 - 2 \cos \omega}} = \epsilon \Psi(\omega),
\] (9)

and are all doubly degenerate. Each pair of solutions consists of a singlet ($S = 0$) and a triplet ($S = 1$) state with opposite Berry [37] (or geometric [38]) phase behavior (Table II). Specifically, if one of the electrons passes once around the ring, the wave function is unaffected in states where $J + S$ is even but changes sign in states where $J + S$ is odd. Two-electron QRs are probably one of the simplest systems that exhibit the Berry phase phenomenon.

In terms of $u$, Eq. (9) is the Heun-like equation [39, 40]
\[
\left( \frac{u^2}{4R^2} - 1 \right) \Psi''(u) + \frac{u}{4R^2} \Psi'(u) + \frac{\Psi(u)}{u} = \epsilon \Psi(u),
\] (10)

with singular points at $-2R$, 0, and $2R$. A Kato-like analysis [41] of (10) yields
\[
\Psi(0) = 0, \quad \frac{\Psi''(0)}{\Psi'(0)} = 1,
\] (11)

which shows that, like $\Psi_{HF}$, $\Psi$ has a node at $u = 0$, and behaves as
\[
\Psi(u) = u \left( 1 + \frac{u}{2} \right) + O(u^3)
\] (12)

for small $u$.

The general solution of (10) is [40]
\[
\Psi^{(a,b)}(u) = u \left( 1 + \frac{u}{2} \right)^{a/2} \left( 1 - \frac{u}{2R} \right)^{b/2} P^{(a,b)}(u),
\] (13)

where $a, b = 0$ or 1, and $P^{(a,b)}$ is a regular power series
\[
P^{(a,b)}(u) = \sum_{k=0}^{\infty} c_k^{(a,b)} u^k.
\] (14)

This produces four families of solutions characterized by the ordered pair $(a, b)$. Substitution of (13) into (10) yields the three-term recurrence relation
\[
c_{k+2}^{(a,b)} = \frac{1}{(k + 2)(k + 3)} \left\{ \left[ \frac{(k + 2)(b - a)}{2R} \right] + 1 \right\} c_{k+1}^{(a,b)} + \frac{k(k + 2 + a + b) + \sigma^{(a,b)}}{4R^2} - \sigma^{(a,b)} \epsilon \right\} c_k^{(a,b)}
\] (15)

with the starting values
\[
c_0^{(a,b)} = 1, \quad c_1^{(a,b)} = \frac{1}{2} \left( 1 + \frac{b - a}{2R} \right).
\] (16)

and
\[
\sigma^{(0,0)} = 1,
\] (17)
\[
\sigma^{(1,0)} = \sigma^{(0,1)} = 1 + 5/(4 - 16R^2\epsilon),
\] (18)
\[
\sigma^{(1,1)} = 1 + 3/(1 - 4R^2\epsilon).
\] (19)

The nodal patterns of the ground state ($i.e.$ single node at $u = 0$) and first excited state (nodes at $u = 0$ and $2R$) are trivial [42], but those of the higher excited states are more complicated, and depend on the value of $R$ (Fig. 2).

Taking (3) as a zeroth-order wave function, one can use standard perturbation theory methods [33] to show that the small-$R$ (weak correlation) expansion of the ground-
TABLE II. Closed-form solutions for the ground and first-excited states of two electrons on a ring.

| $j$ | $n$ | $(a,b)$ | $P_{j,n}^{(a,b)}(u)$ | $R_{j,n}^{(a,b)}$ | $\epsilon_{j,n}^{(a,b)}$ |
|-----|-----|---------|-----------------|-----------------|---------------------|
| 1   | 0   | (1,0)   | $1$             | $1/2$           | $9/4$               |
| 1   | 1   | (0,0)   | $1 + u/2$       | $\sqrt{3/2}$   | $2/3$               |
| 1   | 1   | (1,0)   | $1 + (15 - \sqrt{3})u/24$ | $\sqrt{3(7 + \sqrt{33})/8}$ | $25(7 + \sqrt{33})/96$ |
| 1   | 2   | (0,0)   | $1 + 2u/2 + 5u^2/92$ | $\sqrt{23/2}$ | $9/46$              |
| 2   | 1   | (0,1)   | $1 + (15 + \sqrt{3})u/24$ | $\sqrt{3(7 - \sqrt{33})/8}$ | $25(7 - \sqrt{33})/96$ |
| 2   | 1   | (1,1)   | $1 + u/2$       | $\sqrt{5/2}$   | $4/5$               |
| 2   | 2   | (1,1)   | $1 + u/2 + 7u^2/132$ | $\sqrt{33/2}$ | $5/22$              |

(a) $j = 1$ and $(a,b) = (0,0)$  (b) $j = 1$ and $(a,b) = (1,0)$  (c) $j = 2$ and $(a,b) = (0,1)$  (d) $j = 2$ and $(a,b) = (1,1)$

(e) $j = 3$ and $(a,b) = (0,0)$  (f) $j = 3$ and $(a,b) = (1,0)$  (g) $j = 4$ and $(a,b) = (0,1)$  (h) $j = 4$ and $(a,b) = (1,1)$

(i) $j = 5$ and $(a,b) = (0,0)$  (j) $j = 5$ and $(a,b) = (1,0)$  (k) $j = 6$ and $(a,b) = (0,1)$  (l) $j = 6$ and $(a,b) = (1,1)$

FIG. 2. (Color online) Node positions of closed-form solutions for the ground and excited states of two electrons on a ring. The black lines indicate the position of the non-interacting nodes.

The state ($j = 1$) energy is

$$\epsilon = \epsilon_{HF} - 0.026424 + 0.007241 R - 0.00966 R^2 + 0.000492 R^3 + \ldots$$ (22)

which gives good agreement with the first four values of $R_{j,n}^{(a,b)}$ (Fig. 1). At the other extreme, the large-$R$ (strong correlation) expansion is

$$\epsilon = \frac{1}{2R} + \frac{1}{4R^{3/2}} + \frac{5}{64R^2} + \ldots$$ (23)

Figure 1 reveals that Eq. (23) is accurate over a much wider range of $R$ values than Eq. (22), as one might expect in such a strongly correlated one-dimensional system.

Conclusion.—In this Letter, we have shown that the
Schrödinger equation for two electrons on a ring is solvable in closed form for a countably infinite number of $R$ values. We have demonstrated that, for each value of the angular momentum $J$, one is able to obtain polynomial and irrational solutions for both the singlet and triplet manifolds. The latter are degenerate but exhibit different geometric (Berry) phase behavior. Although, we are not aware of any physical significance for these special values of the radius, they yield exact wave functions in both the weakly and strongly correlated regimes. This makes the present system particularly valuable for testing approximate methods in different correlation regimes. Following the approach developed in this Letter, analytical solutions for other interaction potentials can also be found.

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