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Spin response of impurities in a quantum corral

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In this work we investigate the dependence of spin observables, like the total spin alignment and the spin squeezing factor, for electrons confined inside an elliptic quantum corral and interacting with a pair of impurities located on the semi-major axis of the ellipse. The results suggest that such a system exhibits some of the characteristic features of a qubit, concerning the persistence of the orientation and squeezing of a component of the total spin.

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1. Introduction

The design of quantum computers relies strongly upon practical realization of atomic systems where the information could be kept long enough to be transferred without significant losses. The ultimate realization of such a device would be the measurement of a single-trapped atom. Recently, Moon *et al.* have shown that a single atom, confined to the interior of a quantum corral, can indeed become a control gate for quantum phases. The elliptical resonator of Moon, Lutz and Manoharan, was meant to manipulate degenerate wavefunctions, which are obtained as solutions of Schroedinger equation in a hard-walled ellipse. The same idea was applied by Crommie *et al.*,[2] to investigate the confinement of electrons in quantum corrals on a metal surface. To these works one may add the work of Manoharan *et al.*[3] on the observation of quantum mirages formed by coherent projection of electronic structures consisting of two-dimensional surface state electrons confined in an elliptical quantum corral.

The important results reported by the above mentioned groups[1–3] demonstrate that it would be possible to manipulate quantum states of confined particles.

Therefore, in this context, it may be useful to further explore the properties of quantum corrals, to see the extent to which the manipulation of states preserves, for instance, the orientation of the total spin or its fluctuations along a given direction. The present study aims at the calculation of such properties by assuming that the spin of the confined particles (electrons) interacts with the spin of impurities located in the interior of the quantum corral, with a specific geometry and at a given energy range for the spectrum of the confined electrons.

The theoretical description of static and dynamical properties of quantum corrals has been reported in a series of papers.[4,5] For the purpose of the present work we shall focus on Ref. 3, where the spectral response of electrons placed in an elliptic quantum corral has been investigated. In the work of Ref. 3 the surface electrons (two-dimensional electrons on Cu(111)) were trapped inside a quantum corral made of Co atoms. The motion of the electrons would then be described by single particle states (free-electron gas within an energy band near the Fermi energy) in the interior of the elliptical quantum corral. Like in Ref. 3 we shall assume that the confining atoms are immersed in the electron-sea, and thus they will not appear explicitly in the calculations. In the present scenario we shall not take the interaction of the "free" electrons with the excitations of the electron sea. For each of the associated wavefunctions we shall then restrict our configuration space to these with quantum numbers (and degeneracy) compatible with the actual value of the Fermi energy (see next section).

Motivated by the results of Refs. 1–3 and by the studies of Refs. 4 and 5 we have adopted the techniques developed in our previous works,[6–8] on the atomic response to spin probes, to calculate spin-observables and the spin squeezing factor of a device consisting of confined electrons interacting with a pair of impurities located on the semi-major axis of an elliptical quantum corral. Instead of localized electronic wavefunctions (or spin sites on a lattice) we shall use the wavefunctions resulting from the treatment of the elliptic quantum corral, to calculate the radial integrals appearing in the expectation values of the relevant spin operators. As we shall discuss later on, these wavefunctions are labeled by two quantum numbers, the "radial" quantum number assigned to the number of nodes crossing the semi-minor axis of the ellipse and the "angular momentum" quantum number which counts half the number of nodal intersections along the perimeter corresponding to the "radial" number of nodes.

In order to evaluate spin observables, we have solved the eigenvalue problem of such a system, and selected some of the eigenfunctions. Particularly, we have chosen those wavefunctions whose properties have been reported in Ref. 3, in order to compare our results with some of the experimentally studied configurations of a quantum corral. By this we want to test our results against the ones of Ref. 3, concerning the shapes of the wavefunctions and spacial density distributions, to check the accuracy of the numerical procedure which we have followed to calculate these components of the system. Then, we have calculated the expectation value of the total spin, on the states whose quantum numbers have been determined by the

measured densities,[3] by adding the spin interactions with a pair of impurities placed along the semi-major axis, near the focuses of the elliptical corral, and calculated the spin-squeezing factor and its time evolution. From these results, we have discussed the revival of the spin-squeezing, and the alignment of the total spin.

The details of the formalism are presented in Sec. 2, the results are presented and discussed in Sec. 3, and the conclusions are drawn in Sec. 4.

2. Formalism

We shall begin with the definition of the Hamiltonian, which includes the electronic and impurity degrees of freedom, and solve the eigenvalue problem subject to the boundary conditions of an elliptic corral. As described in the following subsection, we have selected the eigenfunctions which closely reproduce the features shown in Ref. 3 about the spatial density distribution of the confined electrons. Next, we introduce spin observables, like the time evolution of the spin squeezing factor, to study the persistence of the total spin and its fluctuations, depending on the couplings which are contained in the Hamiltonian.

2.1. *The Hamiltonian of the system*

A method for confining electrons to artificial structures has been presented in Ref. 2 and 3. In the work of Ref. 2, 3 surface state electrons on a Cu(111) surface were confined to closed structures, that is quantum corrals of a given geometry, defined by barriers built from atoms.[2,3]

From the point of view of the calculations, to obtain the associated wavefunctions for the confined electrons, we shall define the geometry of the confinement, assumed that it is of the hard-wall type at the boundaries, and that out of the solutions we shall work only with those with eigenvalues near the Fermi surface (determined externally by the density of electrons and by the energy spacing of the spectrum). In this manner we shall avoid further interactions (like particle-hole excitations, pair formation, electron-electron interactions), since we shall deal with these "valence" electrons as free-single-particle excitations. In this respect the approximations are similar to those of other quantum many body systems (like the atomic nuclear problem) where the leading order structure is determined by few free "quasi-nucleons" which can be treated as single-particle excitations of a self-bounded potential, which originates on nucleon–nucleon interactions, neglecting residual particle–particle interactions, particle-vibrations couplings or particle-hole excitations. The works of Ref. 1–3 give a nice example of this realization, together with the set of relevant parameters associated to the picture, some of which have been determined experimentally. In the present context, and speaking about the impurities and other possible scatterers inside the ellipse, taking only the spin interactions and neglecting the Kondo effect, we are referring to the work of Ref. 3 which supports this approximation, since in the words of Ref. 3 removing the Kondo effect along the wall does not influence the essential physics of the quantum mirage.

The Hamiltonian of the system includes the contributions of the electrons and impurities, as well as the interactions among them. The electron-sector of the problem consists of surface-electrons confined to the interior of an elliptical domain with an infinite boundary. The corresponding Schroedinger equation is solved in elliptical coordinates and it yields eigenvalues which can be labeled by the quantum numbers n, which is the number of nodes crossing the semi-minor axis of the ellipse, and l, which is half the number of nodal intersections along the perimeter of the ellipse. Both numbers can be mapped onto the orbital angular-momentum quantum-number in a circle.[9–11] The solutions are ordered by the energy, and we shall select those which are in the proximity of the Fermi energy. Following the results of Refs. 2 and 3 we shall then work with the wavefunctions $\varphi_{n,l}$, which belongs to the states with $n = 4$, $l = 4$ and $n = 2$, $l = 7$. For simplicity, we shall indicate these two configurations by the sub-index α. We shall consider that the two impurities, which are denoted by their spin S_i, are located near the focuses of the ellipse, along it semi-major axis, and that the coupling between the impurities and the spin of the electrons, σ, is weighted by the wavefunctions of the electrons taken at the site of the impurities. The Hamiltonian of the system is written

$$H = H_0 + H_{\rm int}\,, \tag{1}$$

where H_0 is the unperturbed Hamiltonian of the electrons and impurities, and $H_{\rm int}$ is the interaction among them, that is

$$\begin{aligned} H_0 &= \sum_\alpha \epsilon_\alpha (n_{\alpha,\uparrow} + n_{\alpha,\downarrow}) + \sum_i \Delta_i S_i^z\,, \\ H_{\rm int} &= {\rm J} \sum_i \boldsymbol{\sigma}_i \mathbf{S}_i\,, \end{aligned} \tag{2}$$

The electron-spin operators are represented in terms of creation and annihilation operators, weighted by the radial wavefunctions of the electrons $\varphi^*_{i\alpha}$, calculated at the site of the impurities.

$$\begin{aligned} \sigma_i^z &= \frac{1}{2}\sum_{\alpha,\beta} \varphi^*_{i\alpha}\varphi_{i\beta}(c^\dagger_{\alpha\uparrow}c_{\beta\uparrow} - c^\dagger_{\alpha\downarrow}c_{\beta\downarrow})\,, \\ \sigma_i^+ &= \frac{1}{2}\sum_{\alpha,\beta} \varphi^*_{i\alpha}\varphi_{i\beta}c^\dagger_{\alpha\uparrow}c_{\beta\downarrow}\,, \\ \sigma_i^- &= \frac{1}{2}\sum_{\alpha,\beta} \varphi^*_{i\alpha}\varphi_{i\beta}c^\dagger_{\beta\downarrow}c_{\alpha\uparrow} \end{aligned} \tag{3}$$

and

$$n_{\alpha,\uparrow(\downarrow)} = c^\dagger_{\alpha\uparrow(\downarrow)}c_{\alpha\uparrow(\downarrow)}\,, \tag{4}$$

In Eq. (2) the quantities ϵ_α and Δ_i are the energies of the electrons and impurities, and in Eq. (3) the sub-index i indicates that the electron wavefunctions are evaluated at $r = r_i$, which is the site of the impurities. In solving the eigenvalue problem

we have taken advantage of the symmetries of the problem.[9–11] The solutions of the electron-sector of Hamiltonian H_0, are obtained by the diagonalization of the kinetic energy term and the confining one-body potential consisting of an infinite wall located at the borders of the ellipse. They are expanded in the basis of elliptical functions.[9–11] To these solutions we add the interactions between the spin of the electrons and the pair of impurities. Some features of the solutions are discussed next.

2.2. *Eigenvalues and eigenfunctions*

The geometry of the elliptical corral, and the associated coordinates, are sketched in Fig. 1. The coordinates ξ and η are, respectively, associated to radial and angular motion η being perpendicular to the ellipse defined by ξ. $\xi = 0$ represent the horizontal semi-major axis, $\eta = 0$ is the intersection with the positive semi-major axis and for any nonzero value of ξ one has $\eta = \pi/2$, intersection with the semi-minor axis of the ellipse, $\eta = \pi$ is the intersection with the negative semi-major axis of the ellipse, etc. The eigenmodes (two-dimensional standing waves in the interior of the ellipse) are then functions of these two coordinates, and in the notation of regular Mathieu functions,[11] they are identified by the pair of quantum numbers (n, l). As pointed out in Ref. 3 the description advanced so far is supported by the experimental data. Following the same arguments discussed in Ref. 3 we shall look at wavefunctions with correspondence to states near the Fermi energy, and take the corresponding parameters from data.

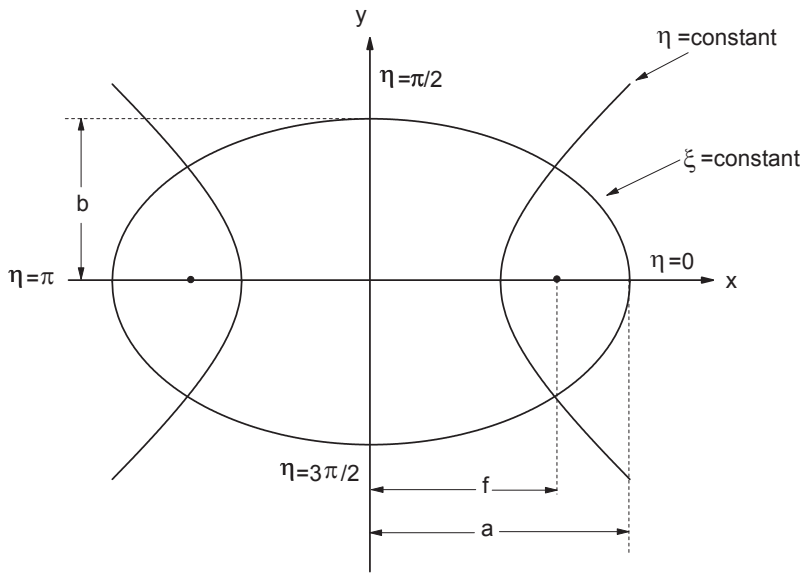

Fig. 1. Coordinates of the elliptical corral; (a) and (b) are the semi-axis of the ellipse, the focuses, radial and angular coordinates are denoted by f, ξ and η, respectively.

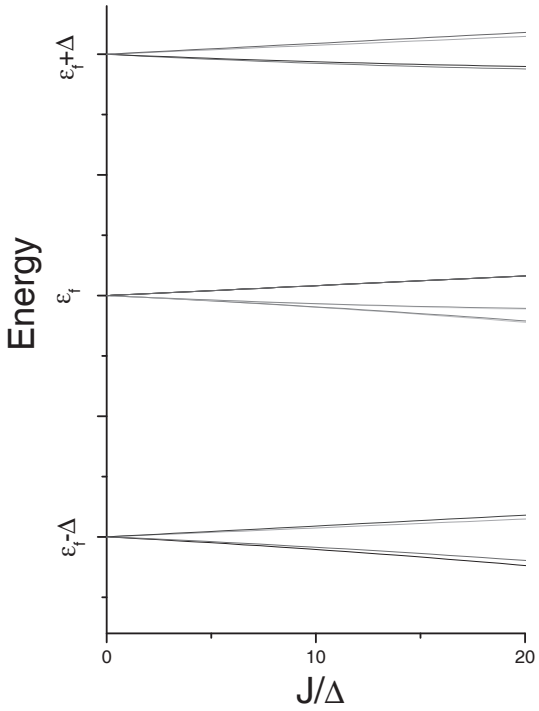

Fig. 2. Eigenvalues of the system near the Fermi energy ϵ_f, as a function of the ratio J/Δ and for $\Delta_i = \Delta$. The impurities are located in an antiparallel configuration (total spin channel $S = 0$) on the major semi-axis, as explained in the text.

The eigenvalues of the Hamiltonian (2), depend on the ratio between the coupling-strengths J and Δ. For simplicity we have taken $\Delta_i = \Delta$. As an example, the dependence of the eigenvalues with the ratio J/Δ, for values in the vicinity of the Fermi energy, is shown in Fig. 2. The configuration corresponding to this spectrum consists of the impurities placed along the major semi-axis of the ellipse, near the focuses, with their spins coupled to total spin $S = 0$ in an antiparallel configuration. The spectrum for the impurities in a parallel array is shown in Fig. 3. As seen from these figures, the degeneracy of H_0 is broken by the interactions between the spin of the electrons and the spin of the impurities. The complexity of the spectrum becomes manifest in the strong coupling limit. There the spectrum becomes increasingly dense, a feature which may be of some relevance for the experimental identification of the states. In the following we shall show the results of the diagonalization of the Hamiltonian, and discuss some features of the adopted wavefunctions. Figures 4 and 5 show the wavefunction and the probability spatial distribution, for four different cases corresponding to values of $(n, l) = (3, 4)$, and $(1, 8)$, and $(n, l) = (2, 7)$, and $(4, 4)$, respectively. The first two configurations are shown for the sake of comparison with the results reported in Ref. 3. These results support the notion that a localized density distribution in the interior of the

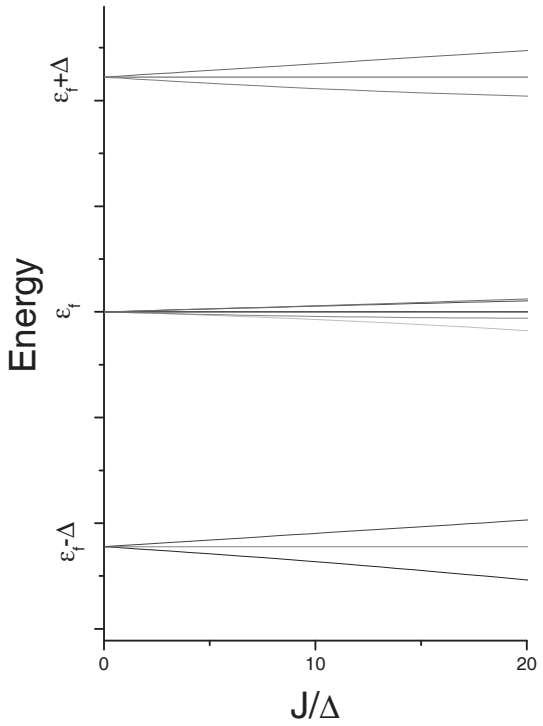

Fig. 3. Eigenvalues of the system, near the Fermi energy ϵ_f, as a function of the ratio J/Δ. The impurities are located in a parallel configuration (total spin channel $S = 1$) on the major semi-axis of the ellipse.

quantum corral, for the impurities in a given configuration, may indeed be obtained by searching for the appropriate eigenvectors. Figure 6 shows the spatial dependence of the wavefunction, along the major axis of the ellipse, for the configurations with $(nl) = (2, 7)$, and $(4, 4)$. The symmetry of the spatial distribution is such that the impurities feel out-of-phase (case $(nl) = (2, 7)$) and in-phase (case $(nl) = (4, 4)$), spatial overlaps in their couplings to the electrons.

2.3. *Spin observables*

Spin squeezed states are quantum states with reduced fluctuations in one of the spin components.[12,13] If $\mathbf{S}_n$ is the spin in the direction of the unit vector $\mathbf{n} \equiv (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$, perpendicular to the direction of the mean value of the total spin $\mathbf{S}$, that is $\langle\mathbf{S}\rangle$. $\mathbf{n} = 0$, then the squeezing factor is defined as[12,13]

$$\zeta^2 = \frac{2(\Delta S_n)^2}{|\langle\mathbf{S}\rangle|}\,, \tag{5}$$

where $(\Delta S_n)^2 = \langle\mathbf{S}_n^2\rangle - \langle\mathbf{S}_n\rangle^2$ is the quadratic deviation of the spin in the direction specified by $\mathbf{n}$. Thus, the expectation value of S_n is squeezed if $\zeta^2 < 1$. The definition

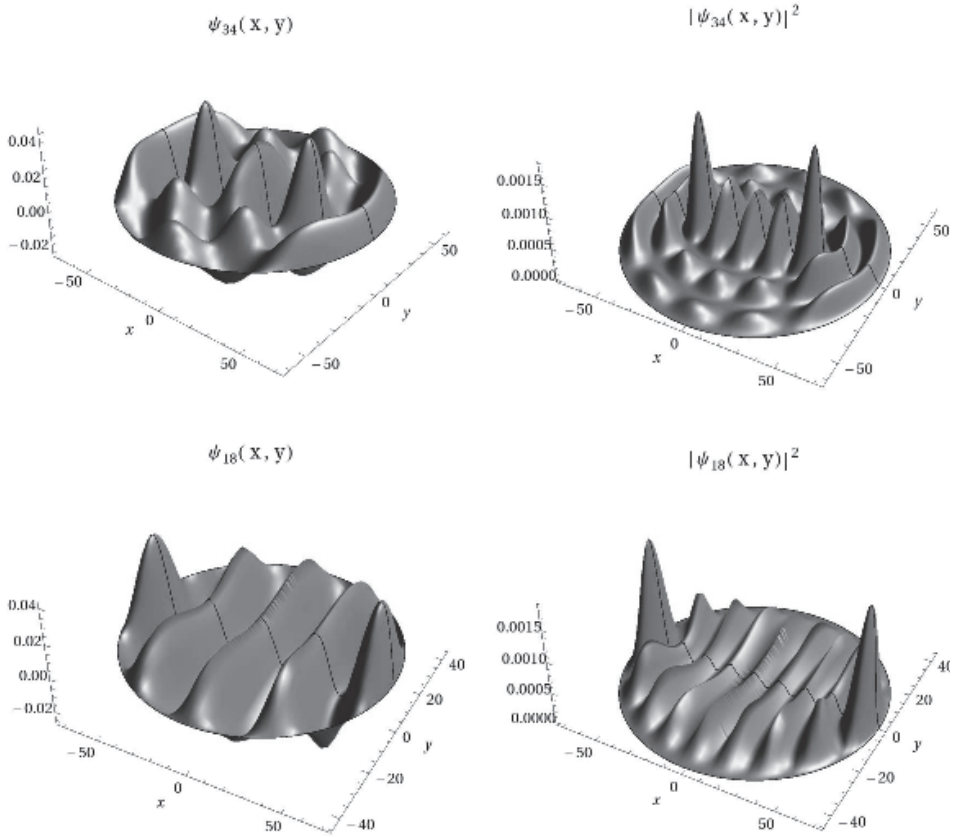

Fig. 4. Spatial amplitude $\psi_{nl}(x,y)$ and probability $|\psi_{nl}(x,y)|^2$, of the configurations with $(nl) = (3,4)$, and $(1,8)$. The coordinates (x,y) are measured along the semi-axis of the ellipse, as shown in the figure.

given in Eq. (5) assumes SU(2) invariance.[14] We are interested in the persistence of the orientation of the spin along the direction defined by the impurities, which are assumed to be aligned by the application of an external field, we shall analyze the time evolution of the quadratic deviation of the component of the total spin along the direction **n**. In this scheme, the optimal squeezing is achieved when the quantum fluctuations of the z-component of the spin are minimal.

In the present calculations we have considered the state

$$\begin{aligned} |I\rangle &= e^{zS_+}|0\rangle\,, \\ z &= e^{-i(\phi_0-\pi)}\tan(\theta_0/2)\,, \end{aligned} \tag{6}$$

as the initial condition. This coherent spin state is not an eigenstate of the Hamiltonian, and it is defined by the orientation angles ϕ_0 and θ_0, of a general unit vector $\mathbf{n} = (\sin\theta_0\cos\phi_0,\, \sin\theta_0\sin\phi_0,\, \cos\theta_0)$. We shall then follow the time evolution of the total spin respect to the direction **n**.[6–8] The operator S_+ is the total

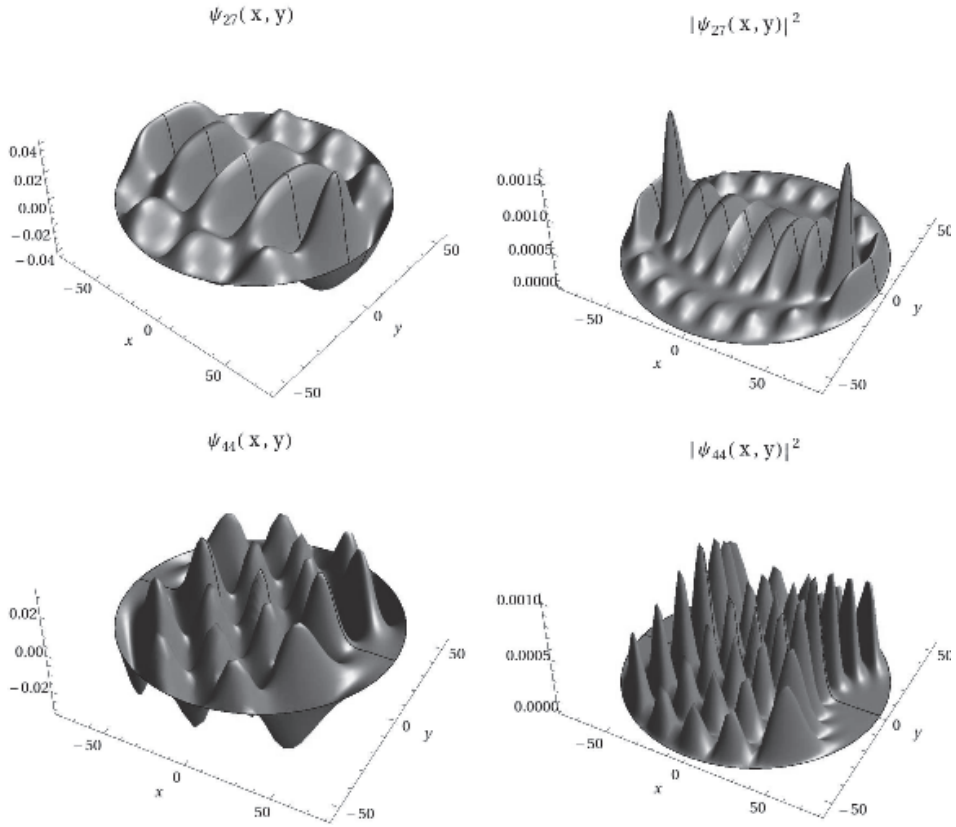

Fig. 5. Spatial amplitude $\psi_{nl}(x, y)$ and probability $|\psi_{nl}(x, y)|^2$, for the configurations with $(nl) = (2, 7)$, and $(4, 4)$.

spin-raising operator $S_+ = \sum_{i=1}^{N} s_{+,i}$, where N is the number of the spin-sites (in this case $N = 2$).

In the basis of eigenvectors of H, the time evolution of a given operator O is expressed as[6–8]

$$O(t) = U^\dagger(t) O U(t), \quad U(t) = e^{-iHt/\hbar}. \tag{7}$$

The expectation value $\langle O(t)\rangle$ is then written

$$\begin{aligned} \langle O(t)\rangle &= \mathrm{Tr}(\rho(t)O) \\ &= \sum_{\beta,\gamma} \langle\gamma|I\rangle\langle I|\beta\rangle\langle\beta|O|\gamma\rangle e^{-i(E_\beta - E_\gamma)t/\hbar}, \end{aligned} \tag{8}$$

where we have defined the density operator $\rho(t) = U^\dagger(t)\rho(0)U(t)$, being $\rho(0) = |I\rangle\langle I|$; the state $|I\rangle$ is the initial state, while $\{E_\beta\}$ and $\{|\beta\rangle\}$ are the βth eigenvalue and eigenvector of the total Hamiltonian.

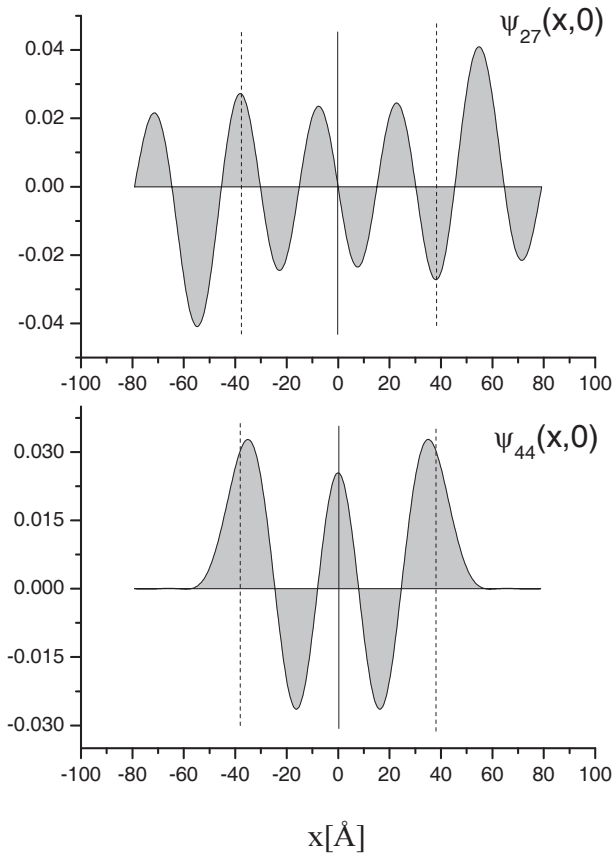

Fig. 6. wavefunctions along the major axis (the x-axis) of the ellipse, for two different pair of quantum numbers (n, l). The position of the impurities is shown by vertical dashed-lines.

The expression (8) can be written in a more compact form in terms of the overlap of the initial state $|I\rangle$ with the eigenvectors $\{|\beta\rangle\}$, that is[7]

$$\begin{aligned} \langle O(t)\rangle &= \sum_{n,m} T^*(n)\langle n|O|m\rangle T(m)\,, \\ T(m) &= \sum_{\beta n} c^*_{\beta n} c_{\beta m}\langle n|I\rangle e^{iE_\beta t/\hbar}\,. \end{aligned} \tag{9}$$

In the above equation $|n\rangle$ is an element of the basis, and the coefficient $c_{\beta n}$ is the amplitude of $|n\rangle$ in the eigenstate $|\beta\rangle$ of the Hamiltonian.

3. Results and Discussion

The dimensions of the confining, elliptic quantum corral are fixed at the values $a = 78.5$ Å, and $b = 55$ Å, for the semi-axis of the ellipse, $e = 1.42$ for the eccentricity, and the parameters of the interaction are taken from Ref. 3. The resulting

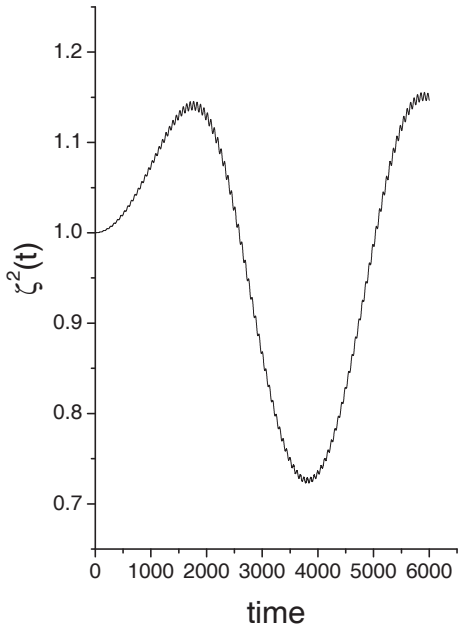

Fig. 7. Spin-squeezing factor, ζ^2, calculated for the spectrum of Fig. 2, as explained in the text, and for impurities placed, on the major semi-axis, near the focuses of the ellipse ($x_f = \pm 38.2$ Å). The time is measured in units of inverse-energy (since $\hbar = 1$).

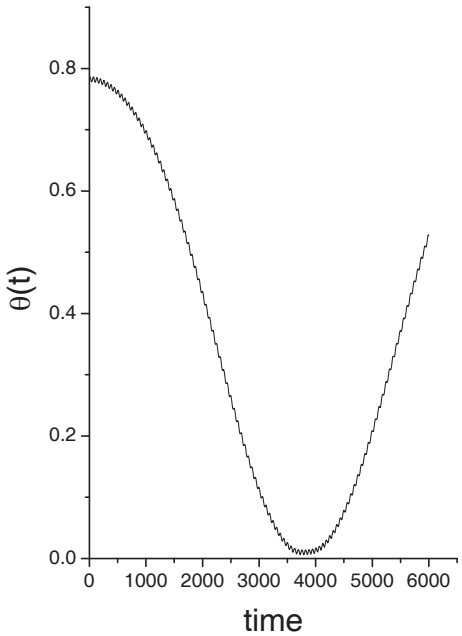

Fig. 8. Time dependence of the polar orientation angle, $\theta(t)$, associated to the results shown in Fig. 7.

Fermi energy is of the order of 445 meV, and the electron effective mass was fixed at the value $m^*/m_0 = 0.38$. The coupling constant J was varied between 0 meV and 10 meV, and the gap Δ was fixed at the value $\Delta = 1$ meV. With the obtained eigenvectors we have constructed the density matrix needed to calculate the expectation value of a given operator. The technique is rather simple, it has been presented in detail in Refs. 6–8, and we shall avoid repeating it here. Figure 7 shows the time evolution of the squeezing factor obtained by using the eigenvalues and eigenvectors corresponding to the spectrum of Fig. 2. The results correspond to calculations performed with the parameters $J = 0.1$, and $\Delta = 1$ meV. The amplitudes of the electron-wavefunctions at the site of the impurities are the ones shown in Fig. 6. Concerning the squeezing, see Fig. 7, it becomes manifest with a pattern of revival with a first minimum at t ≈ 4000, which is correlated with the minimum of the orientation angle θ. This is supported by the results shown in Fig. 8, where the polar angle reaches a vanishing value at the same time $t \approx 4000$. It is seen, from the time evolution of the polar angle $\theta(t)$, that the fluctuations of the standard deviation of the spin in the direction of $\mathbf{n}$ are minimized for an average orientation angle $\bar{\theta}(t) \approx \pi/8$. The time dependence of the polar angle coincides with the pattern of revival of the spin squeezing factor. In Figs. 7 and 8 the time is given in units of inverse-energy, since we have adopted the value $\hbar = 1$ consistently in the calculations.

4. Conclusions

In this work we have calculated the spectrum of a system of confined electrons and impurities, with the boundary conditions of an elliptic quantum corral. We have searched for signals of the persistence of the orientation of the total spin of the system. We found a definite degree of squeezing, which is correlated with a sharp spin orientation at zero polar angle and which displays a clear pattern of revival. These results depend on the position of the impurities, the adopted wavefunctions and the strength of the couplings. However, as we have verified in performing the calculations, it is indeed possible to find out a set of highly localized spacial density distributions for which the spin squeezing phenomena may appear. The time dependence of the calculated spin squeezing factor shows a pattern of revival. The time scale of the revival is then fixed by the strength of the couplings between the impurities and the electrons, as well by the density of eigenvalues of the Hamiltonian. However, since the Kondo effect has not been considered, the spin orientation and squeezing found in the present calculations may be affected and/or competing with the spin polarization eventually produced by the Kondo resonance, as suggested in Ref. 3.

Acknowledgments

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References

1. C. R. Moon, C. P. Lutz and C. H. Manoharan, *Nature Phys.* **4**, 454 (2008).
2. M. F. Crommie, C. P. Lutz and D. M. Eigler, *Science* **262**, 218 (1993).
3. C. H. Manoharan, C. P. Lutz and D. M. Eigler, *Nature* **403**, 512 (2000).
4. M. Nizama, K. Hallberg and J. d'Albuquerque e Castro, *Phys. Rev. B* **75**, 235445 (2007).
5. M. Nizama, D. Frustaglia and K. Hallberg, *Physica B* **404**, 2819 (2009).
6. M. Reboiro, O. Civitarese and D. Tielas, *J. Phys. B* **46**, 065502 (2013).
7. O. Civitarese *et al.*, *Phys. Lett. A* **373**, 754 (2009).
8. O. Civitarese *et al.*, *Phys. Lett. A* **374**, 2117 (2010).
9. M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions* (Dover, New York, 1965).
10. R. van Zon and Th. W. Ruijgrok, *Eur. J. Phys.* **19**, 77 (1998).
11. J. C. Gutierrez Vega *et al.*, *Am. J. Phys.* **71**, 233 (2003).
12. M. Kitagawa and M. Ueda, *Phys. Rev. A* **47**, 5138 (1993).
13. D. J. Wineland *et al.*. *Phys. Rev. A* **46**, 11 (1992).
14. A. Luis and N. Korolkova, *Phys. Rev. A* **74**, 043817 (2007).