Nonlinear Schroedinger-Poisson Theory for Quantum-Dot Helium

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We use a nonlinear Schroedinger-Poisson equation to describe two interacting electrons with opposite spins confined in a parabolic potential, a quantum dot. We propose an effective form of the Poisson equation taking into account the dimensional mismatch of the two-dimensional electronic system and the three-dimensional electrostatics. The results agree with earlier numerical calculations performed in a large basis of two-body states and provide a simple model for continuous quantum-classical transition with increasing nonlinearity. Specific intriguing properties due to eigenstate non-orthogonality are emphasized.

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I. INTRODUCTION

Quantum-dots can be viewed as artificially structured atoms in heterojunctions or metal-oxide-semiconductor devices where few electrons are confined to a length comparable to the mesoscopic effective Bohr radius \( a_B \) (\( a_B \approx 10^{-2} \) \( \mu m \) in the case of GaAs). Though the confinement can \textit{a priori} occur in all three directions, some types of experimentally realized quantum-dots display an extension in the \( x-y \) plane which is much larger than in the growth direction \( z \) of the underlying semiconductor structure.\(^{2,3}\) Therefore, these quantum-dots are usually regarded as artificial atoms with a disk-like shape. Since electron numbers \( N \) as low as one or two per dot have already been realized,\(^{1}\) quantum-dot Helium consisting of two electrons trapped in the two-dimensional (2D) axisymmetrical harmonic potential \( V(r) = \frac{1}{2} M \omega^2 r^2 \), where \( r^2 = x^2 + y^2 \) and \( M \) is the effective electron mass, is actually considered as the simplest realistic model for an interacting quantum system.\(^{4,5}\) As itself or amongst other such few-electron systems, it has been extensively studied in the relationship with the development of nanotechnologies.\(^{6,7,8,9}\) Both its exact 2D-3D analytical\(^{6,7}\) or 2D numerical solutions in the presence of a perpendicular homogeneous external magnetic field are known, in particular by use of the separation of the Hamiltonian into its center-of-mass and relative-motion terms, due to the assumption of a parabolic particle confinement. Oscillations between spin-singlet and spin-triplet ground states as a function of the magnetic field strength have been predicted\(^{10}\) and experimentally observed.\(^{11}\) They are due to the interplay between the dot size and the strength of the magnetic field. Another important competition occurs between the kinetic-energy matrix elements and the electron-electron Coulomb interaction ones when changing the characteristic length \( L \) of the quantum dot without changing its shape. Indeed, for small \( L \), the Coulomb interaction becomes negligible and the electrons behave like independent, uncorrelated particles.\(^{12}\) This happens in particular in the case of strong parabolic confinement \( \omega \rightarrow \infty \) since then \( L \sim l_0 = \sqrt{\hbar/M \omega} \rightarrow 0 \).

In this rich theoretical and experimental context, we wish to emphasize new physical results by use of a quite original – with respect to the above state of the art – differential approach based on the Schroedinger-Poisson (SP) definition of single-particle nonlinear eigenstates in quantum-dot Helium. The problem with such eigenstates is that, being the (stationary) solutions of the SP nonlinear differential system, they are not orthogonal. The whole matrix machinery of quantum mechanics then fails and we are left to return to its \textit{ab-initio} fundamental principles. In particular, the square scalar product \( P = |\Psi_a| \Psi_b|^2 \neq 0 \) of two such nonlinear eigenstates \( \Psi_a \) and \( \Psi_b \) defines the probability to find the system in either state when it is known to be in the other one (this probability is of course zero for orthogonal Hilbertian eigenstates). Equivalently – and this will be precisely shown below by use of the Fermi golden rule –, \( P \) yields the transition probability either from \( \Psi_a \) to \( \Psi_b \) or reverse. Therefore, if \( \Psi_a \) is, say, the fundamental eigenstate and \( \Psi_b \) is an excited one, \( P \) either measures the probability of an absorption process \( (\Psi_a \rightarrow \Psi_b) \) or an emission one \( (\Psi_b \rightarrow \Psi_a) \). The following couple of questions are then addressed and tentative answers provided: i) What energy is actually absorbed or emitted as a consequence of the non-orthogonality of the nonlinear eigenstates \( \Psi_{a,b} \)? ii) Are the affiliated energy exchanges quantized and how?

The present paper is built as follows. We first display, by use of standard numerical tools\(^{13}\) the remarkable properties of the solutions \{\( u_N \), \( C_N \)\} of the SP dimensionless nonlinear differential system, where \( N \) is the nonlinear control parameter whose value is given by the harmonic trap parabolicity \( \omega \). Then we numerically investigate the square scalar product \( P_{1,3} = |u_{1,3}|^2 \neq 0 \) of its first two (zero-angular-momentum, for the sake of simplicity) eigenstates \( u_{1,3} \) when \( N \) is increased. Subscripts always refer, in the present work, to those single-particle energy eigenvalues (in units of \( \hbar \omega \)) which correspond to the \( N \rightarrow 0 \) linear limit. We find an interference-like pattern \( \propto \sin^2 \left( \frac{\pi}{2} N \right) \). Then we validate the above results both by stressing the link between \( P_{1,3} \) and Fermi’s golden rule for small nonlinearity \( N \leq 1 \), as well as by displaying the transition of the system to the asymptotic
semi-classical Thomas-Fermi regime for high values of the nonlinearity $\mathcal{N} \gg 1$. Finally, we test the reliability of the present SP description of quantum-dot Helium by comparison with the existing numerical (Refs [1] & [2], respectively Figs 1 and 3) and analytical (Ref. [8]: Fig. 1b) data concerning either the fundamental energy level or, like in Ref. [9], its (electro)chemical potential. In all cases our nonlinear SP eigensolutions do agree surprisingly well (i.e. within the percent) with the existing numerical results, is defined by

$$\mathcal{N} \equiv \mathcal{N}(\omega)$$

We have: 

$$\mathcal{N} = \frac{\hbar \omega}{2C_0}$$

The corresponding dimensionless parameter $\tilde{\mathcal{N}} = \mathcal{N}(\omega)$ will be defined below and is a typical measure of the SP nonlinearity. It is important to keep in mind that the above system Eqs (42) is only relevant for particles in the same orbital state $\Psi$. 

Assuming the 2D axisymmetrical parabolic confining potential $V(x, y) = V(r) = \frac{1}{2}M\omega^2 r^2$, we have:

$$\Psi(x, y) = \Psi(r, \phi) = \psi(r) e^{im\phi}.$$ (3)
Here
\[ u^{\text{lin}}(X) \propto e^{-\frac{X^2}{2}} X^2 P_n(X), \tag{8} \]
defines the \( N \to 0 \) linear solutions in terms of the quantum numbers \( n \) and \( m \) and of the Laguerre polynomial \( P_n(X) \), namely \( P_0 = 1; P_1 = 1 - \frac{1}{2}X^2; P_2 = 2 - 2X^2 + \frac{1}{3}X^4; P_3 = 6 - 9X^2 + \frac{5}{4}X^4 - \frac{1}{6}X^6 \ldots \) These single-particle linear parabolic states correspond to the energy eigenvalues
\[ E^{\text{lin}} = E_{n,m} = (2n + |m| + 1) \hbar \omega. \tag{9} \]

Figure 1 displays the \( C_0 \) versus \( u_0 \) spiraling trajectories for the two first \( m = 0 \) eigenstates \( u_1 \) (circles) and \( u_3 \) (stars). Recall that the subscripts always refer in the present work to the number of \( \hbar \omega \) quanta present in the \( N \to 0 \) linear limit of the single-particle energy, in accordance with Eq. 9. These trajectories in the \( \{u_0, C_0\} \) plane are parametrized with respect to increasing values of the nonlinear parameter \( N \), i.e., with decreasing values of the trap harmonicity \( \omega \). Indeed electron-electron interaction becomes relatively (with respect to quantum kinetic energy) more and more important when the two electrons are less and less confined (see above Part I). Actually \( N \) varies in Fig. 1 from \( 10^{-2} \) (\( u_0 \sim 0.1 \)) to \( 10^2 \) (\( u_0 \sim 1 \)) where one then reaches the quasi-classical asymptotic Thomas-Fermi regime. This regime is defined by neglecting the quantum kinetic derivative terms in Eq. (4a), thus yielding \( C(X) \sim X^2/4 \) and hence \( C_0 = C(0) = 0 \), while \( u(X) \equiv 1 \) through Eq. (4b). Therefore the initial conditions for the two discrete modes \( u_1 \) and \( u_3 \) converge towards the Thomas-Fermi fixed point \( \{u_0 = 1; C_0 = 0\} \) for \( N \to \infty \) as evidenced by Fig. 1. Physically, this means that there is a continuous transition, through the increase of nonlinearity in the system, from the \( N \leq \pi \) “pure” quantum regime where the quantum kinetic energy defined by the derivative terms in Eq. (4a) plays a major role towards the \( N \to \pi \) classical one where the dimensionless Schroedinger equation Eq. (4b) reduces to its last-bracket classical-energy term. As a consequence, the \( N \to \infty \) highly nonlinear case leads to the progressive merging of the two discrete energy levels \( u_1 \) and \( u_3 \) into the single one whose initial conditions are defined by the fixed point displayed in Fig. 1. Therefore quantum eigenstate discreteness disappears, which is the hallmark of the classical regime: a continuous energy spectrum sets on about the uniform wavefunction profile \( u(X) \equiv 1 \) and \( C(X) \equiv 0 \), where the chemical potential equals the – here vanishing, due to our \( m = 0 \) assumption – centrifugal potential plus the electrostatic interaction potential, as shown by Eq. (5). The onset of the first corresponding oscillation in the amplitude of the respective modes \( u_1(X) \) (continuous line) and \( u_3(X) \) (dotted line) is displayed in Fig. 2.

![Figure 1](image1.png)

**FIG. 1:** (Color online). The convergence of the discrete SP nonlinear system towards the quasi-classical continuum Thomas-Fermi regime defined by the fixed point \( u \equiv 1 \) and \( C_0 = \frac{1}{2\pi} X^2 |X = 0| = 0 \) when \( N \) increases from \( \sim 10^{-2} \) to \( \sim 10^2 \) in the \( \{C_0 \text{ vs } u_0\} \) boundary condition phase space for the two first \( m = 0 \) nonlinear eigenmodes defined by their corresponding linear quantum numbers: namely (cf. Eq. 9) \( n = 0, m = 0 \) (\( u_1 \): circles) and \( n = 1, m = 0 \) (\( u_3 \): stars).

![Figure 2](image2.png)

**FIG. 2:** (Color online). Several nonlinear eigenstate profiles \( u_1(X) \) (continuous line) and \( u_3(X) \) (dashed line) for increasing values of the dimensionless quantum-dot size \( k \), namely \( 10^{-2} \leq k \leq 8.7 \), where \( k = l_0/a^* \) is the ratio of the characteristic harmonic length \( l_0 = \sqrt{\hbar / M \omega} \) over the effective Bohr radius \( a^* = \hbar^2 / Me^2 \). The maximum-amplitude thresholds at \( u_0 \sim 1.2 \) (resp. \( u_0 \sim 1.8 \)) for the ground-state mode \( u_1 \) (resp. the excited mode \( u_3 \)) and displayed by Fig. 1 are clearly visible (profile accumulation effect).

IV. CHEMICAL POTENTIAL AND ENERGY: THE EXPLICIT DEFINITION \( N(\omega) \)

In the following, we shall only consider zero-angular-momentum \( m = 0 \) states for the sake of simplicity (we have indeed checked that \( m \neq 0 \) nonlinear eigenstates are
equally well described by the above differential system: see below Fig. 4 where the quantum-dot spectra are displayed versus their corresponding \( N \) for \( n \leq 3; m \leq 3 \). The SP virial energy \( E \) per particle corresponding to the nonlinear eigenstate \( u(X) \) is twice the expectation value \( \langle \frac{1}{2} M \omega^2 r^2 \rangle \) of the external parabolic potential energy (virial theorem for a harmonic potential). In terms of the dimensionless quantities defined in Eqs (9), it reads

\[
\hat{E} = \frac{1}{2N} \int_0^\infty u^2 X^3 dX.
\]  

(10)

On the other hand, the chemical potential \( \mu \) defined by Eq. (1) is that energy which is required in order to add the second electron to the single-electron quantum-dot (Koopman’s theorem). It can truly be regarded as the nonlinear eigenvalue of the SP differential system related to the corresponding nonlinear eigenstate \( \Psi \) (or \( u \) in the reduced units defined in Eqs (5)). Therefore we have

\[
\hat{\mu} = 2\hat{E} - \hat{E}^{\text{lin}},
\]

(11)

where \( E^{\text{lin}} = E_{n,m} \) is defined by Eq. (6). In the present work where we only consider \( m = 0 \) eigenstates, the two first levels are \( \hat{E}_1 \) (resp. \( \hat{E}_3 \)) corresponding to \( n = 0 \) (resp. \( n = 1 \)) in units of \( \hbar \omega \). The nonlinear integrodifferential system Eqs (4) is closed by the use of Eq. (5) at \( X = 0 \). This yields the (reduced) chemical potential \( \hat{\mu} = \mu / \hbar \omega \) for \( m = 0 \)

\[
\hat{\mu} = C(0) + \frac{e^2}{\hbar \omega} \int \frac{|\Psi|^2}{r} d^3x
\]

\[
= C_0 + \frac{\sqrt{\hbar}}{N} \int_0^\infty u^2 dX,
\]

(12)

where \( k = l_0 / a^* \) is the usual dimensionless dot size corresponding to the harmonic length \( l_0 = \sqrt{\hbar / M \omega} \) and the effective Bohr radius \( a^* = \hbar^2 / M e^2 \) (ranging from \( a^* = 67 \text{ nm} \) for InSb to \( a^* = 9.8 \text{ nm} \) for GaAs).

Equations (11) self-consistently define, for any given value of the trap characteristic harmonic frequency \( \omega \) (or, equivalently, its reduced size \( k \)), the solution \( u = u_\omega(X) \), its norm \( \bar{N} = N(\omega) \) as well as its corresponding single-particle energy \( \hat{E} = \hat{E}_\omega \) (together with the chemical potential \( \hat{\mu} = \mu_\omega \)). We numerically obtain, for instance the ground state in the “quantum-regime” interval of values \( N \leq \pi \) (see below)

\[
\bar{N}(k) \sim \frac{0.8839 k}{0.4218 + 0.1247 k}
\]

(13)

while its energy is

\[
\hat{E}(N) \sim 1 + 0.24670 N + 0.03683 N^2 - 0.00217 N^3.
\]

(14)

Therefore \( \bar{N}(k) \) is a monotonic increasing function of the dot size, starting like \( \bar{N} \sim 2k \) for small values of the dot size \( k \), while

\[
\hat{E} \sim \hat{E}_{\text{lin}} + \frac{1}{4} N \quad \Theta \quad N < 1 \quad \leftrightarrow \quad k < \frac{1}{2}
\]

(15)

In Ref. 5, for instance, where \( \hbar \omega = 3.37 \text{ meV} \) for a GaAs parabolic quantum dot (\( M \) equals 0.067 electron mass while the charge is 1/\( \sqrt{12.4} \) electron charge), we have \( a^* = 9.79 \text{ nm} \) and \( l_0 = 18.5 \text{ nm} \). Hence \( k = 1.89 \). Then Eqs (13) respectively yield \( N = 2.53 \) and \( \hat{E} = \hat{E}_{\text{per} \text{ particle}} = 1.83 \). Therefore \( E_{\text{quantum dot}} = 2 \hat{E}_{\text{per} \text{ particle}} = 2(1.83) \hbar \omega = 12.33 \text{ meV} \) to be compared with PGM’s value 12.28 meV: see Fig. 3 where the virial energy per particle (solid line), defined by Eq. (10), is plotted together with the Koopman one (dashed line), defined from Eqs (9). The energy per particle \( \hat{E} \) is defined by the intersection of both plots. Similarly, in

![Graph showing the chemical potential and energy per particle for a GaAs quantum-dot Parahelix defined by the confinement \( h \omega = 3.37 \text{ meV} \), the dielectric constant of the bulk material \( \kappa = 12.4 \) and the effective mass \( M = 0.067 m_e \) where \( m_e \) is the electron mass.](image)

FIG. 3: (Color online). For GaAs quantum-dot Parahelix defined by the confinement \( h \omega = 3.37 \text{ meV} \), the dielectric constant of the bulk material \( \kappa = 12.4 \) and the effective mass \( M = 0.067 m_e \) where \( m_e \) is the electron mass, we have \( N = 2.53 \) and \( \hat{E} = 1.83 \) by use of (respectively) Eqs (13) & (14). This last SP ground-state energy per particle value appears here as the intersection of its virial (continuous line) and its Koopman (dashed-dotted line) definitions as respectively provided by Eqs (10) & (11). PGM’s exact numerical value \( \hat{E} = \frac{1}{2}(12.28) \text{ meV} / 3.37 \text{ meV} = 1.822 \) given in Ref. (5) is plotted as the horizontal segment.

Ref. 8, \( \hbar \omega = 2 \text{ meV} \) yields \( k = 2.43 \). Hence \( N = 2.97 \) and \( \hat{E} = 2.00 \), which yields \( \hat{\mu} = 2\hat{E} - 1 = 3.00 \) in accordance with Eq. (11), and therefore \( \mu = 3.00 \hbar \omega = 6.00 \text{ meV} \) which is in complete agreement with the Coulomb-interaction case (\( d_1 = d_2 = \infty \)) of that reference.

A remarkable property of the SP nonlinear eigenisolutions is their “universal” limit behavior defined by Eq. (15) for small \( N \), whatever the actual state’s quantum numbers \( n \) and \( m \) in Eq. (4): see Fig. 4 where \( \hat{E} = \hat{E}_{\text{lin}} + \frac{1}{4} N \) is plotted in dashed line. Therefore the energy

\[
\Delta = \frac{1}{2} N \hbar \omega,
\]

(16)

which was introduced for dimensional reasons into the Poisson equation (2) is simply the smallest additional
quantum-dot energy due to particle-particle interaction nonlinearity. Indeed Eq. (15) yields for the $2E$ quantum-dot energy

$$\lim_{N \to 0} 2E = 2E^{\text{lin}} + \Delta,$$

(17)

where $E^{\text{lin}}$ is the $N = 0$ linear energy per particle defined by Eq. (9). Therefore $\Delta$ is the smallest interaction (or nonlinear) energy value in our two-electron SP system that comes in addition to the already existing "linear" quanta $\hbar \omega$, when $N \to 0$. To see whether $\Delta$ is a true "nonlinear quantum" of energy – i.e. whether the energy exchanges between the two levels $E_1$ and $E_3$ can be described in the terms of both $\hbar \omega$ and $\Delta$ – demands to define the actual transition probability between these levels from the non-orthogonality of the corresponding eigenstates. This will be done in the next part.

V. THE SCALAR PRODUCT $\langle u_1|u_3 \rangle$ AND THE CORRESPONDING TRANSITION PROBABILITY

Let us define the (normalized) scalar product

$$\langle u_1|u_3 \rangle = \frac{1}{\sqrt{N_1N_3}} \int_0^{\infty} u_1u_3 \, X \, dX,$$

(18)

together with

$$\begin{align*}
\int_0^{\infty} u_1^2 X^3 \, dX - N_1 (1 + C_{(1)}^0) &= \int_0^{\infty} u_1^2 \, dX \\
\int_0^{\infty} u_3^2 X^3 \, dX - N_3 (3 + C_{(3)}^0) &= \int_0^{\infty} u_3^2 \, dX,
\end{align*}$$

(19)

defined by Eqs (15) which states that the trap harmonicity $\omega$, or equivalently its quantum-dot dimensionless length $k = \sqrt{\hbar/M\omega/(\hbar^2/M \omega^2)}$, must be identical for the two modes $u_{1,3}$ that enter the calculation of the scalar product $\langle u_1|u_3 \rangle$. Practically, in the numerical simulations of Eqs (18-20), we will consider Eq. (19) as verified if it is fulfilled within an $10^{-6}$ error.

In order for the scalar product Eqs (18-20) to make physical sense, we wish to link it with standard time-independent linear perturbation theory in the case of small nonlinearity $N' \ll 1$, i.e. for small "perturbative" particle-particle interaction $\Phi$ defined by Eqs (11-12). Therefore we deduce that

$$\lim_{N' \to 0} \langle u_1|u_3 \rangle^2 = \mathcal{P}_{1,3},$$

(21)

where

$$\mathcal{P}_{1,3} = \frac{4}{\hbar^2} |\langle u_3^{\text{lin}} | H^{\text{pert}} | u_1^{\text{lin}} \rangle|^2 \frac{\sin^2(\frac{1}{2} \omega_{13} t)}{\omega_{13}^2},$$

(22)

together with $\hbar \omega_{1,3} = E_3 - E_1 \sim 2\hbar \omega$, yields Fermi golden rule’s transition probability per particle. Indeed both the energies $E_i \sim E_{\frac{3}{2}(i-1),0}$ per particle ($i = 1, 3$; cf. Eq. (9)) and the corresponding normalized eigenstates $u_i \sim u_i^{\text{lin}}$ in Eq. (22) are those corresponding to the unperturbed linear system (hence the superscript), namely $u_1^{\text{lin}} = e^{-X^2/4}$ and $u_3^{\text{lin}} = (1 - \frac{X^2}{2})e^{-X^2/4}$ (cf. Eqs (9)). The perturbation potential $H^{\text{pert}}$ is equal to $\frac{1}{2} \Phi$ (per particle: hence the factor $\frac{1}{2}$) where $\Phi = \frac{1}{2} [\Phi^{(1)} + \Phi^{(3)}]$ is the interaction potential that has been averaged over its two components $\Phi^{(1)}$ and $\Phi^{(3)}$. Therefore

$$\langle u_3^{\text{lin}} | H^{\text{pert}} | u_1^{\text{lin}} \rangle = H_{13}^{\text{pert}} = \frac{1}{2} [\ddot{\Phi}_{13}],$$

(23)

where the matrix elements $\ddot{\Phi}_{13}^{(i)} (i = 1, 3)$ have been calculated by use of the above-mentioned linear normalized eigenstates $u_{1,3}^{\text{lin}}$. In the stationary perturbative regime where $\omega_{1,3} t \sim 2\omega t \gg 1 \gg H^{\text{pert}}/\hbar$, the time-dependent
term in Eq. (22) can be replaced by its averaged value \( \frac{1}{3} \), yielding \( P_{13} = \frac{1}{2} [\tilde{H}_{13}^{\text{pert}}]^{2} = \frac{1}{32} [\tilde{\Phi}_{13}^{(1)} + \tilde{\Phi}_{13}^{(3)}]^{2} \). Therefore Eq. (21) becomes

\[
\lim_{N \to 0} \frac{N}{2} = \lim_{N \to 0} \left[ \frac{\tilde{\Phi}_{13}^{(1)} + \tilde{\Phi}_{13}^{(3)}}{2} \right] = 2\sqrt{2} |\langle u_{1}|u_{3}\rangle|. \tag{24}
\]

Figure 5 displays the r.h.s. of Eq. (24) (continuous line) versus its l.h.s. (dashed-dotted line) and shows the numerical fulfillement of this condition.

Therefore the square scalar product defined by Eqs (19-22) yields, in the limit of small nonlinearity \( N_{1,3} \), the transition probability \( P_{13} \) from the fundamental nonlinear eigenstate \( u_{1} \) to the excited one \( u_{3} \) or reverse. On the other hand, we showed in Section III that the quasiclassical Thomas-Fermi regime yields \( \lim_{N \to 0} u_{1,3} \equiv 1 \) (see Fig. 1). The two modes \( u_{1,3} \) then become equivalent. Consequently the transition probability between them should obviously become equal to unity, which is consistent with \( (\langle u_{1}|u_{3}\rangle)^{2} \}_{u_{1} \sim u_{3}} = 1 \) from definition (13). Therefore it seems quite natural to extrapolate to all values of the nonlinearity \( N_{1,3} \) the physical meaning of \( \langle u_{1}|u_{3}\rangle^{2} \) in terms of the transition probability \( P_{13} \) as defined by Eqs (21-22).

\[ V_{\text{mean}} - V_{\text{field}} \text{ potentials in units of } \hbar \omega \]

\[ \Delta_{N} = \Delta_{N_{1}} \sim \pi \]

VI. QUANTUM TRANSITIONS BETWEEN TWO \( m = 0 \) NONLINEAR EIGENSTATES

Let us now proceed to the investigation of the quantum transitions between the two nonlinear eigenstates \( u_{1,3} \) by use of the numerical calculation of the scalar product defined by Eqs (18-20). It consists in increasing the nonlinearity through a three-loop iterative scheme from the \( N \ll 1 \) linear regime. The two first loops define each eigenstate \( u_{1,3} \) which vanish with a \( 10^{-7} \) accuracy at \( X \sim 9 \) which is our numerical value for \( X \sim \infty \) (see Fig. 2) while the third one evaluates the matching condition Eq. (19) within \( 10^{-6} \) and then calculates the scalar product given by Eq. (18). The integrals which appear in Eqs (18-20) are transformed into additional first-order ordinary differential equations with vanishing initial conditions whose solutions are taken at \( X \sim 9 \). Then the whole resulting differential system is numerically integrated by use of standard tools.

Figure 6 displays the following remarkable interference-like pattern with respect to the ground-state nonlinear parameter \( N_{1} \). Intriguing enough, since the present SP differential model is non-relativistic (there is no velocity of light in it), it is best scaled by use of the numerical value of the fine-structure-constant \( \alpha = e^{2}/\hbar c \) multiplied by \( \pi \), namely \( \pi/137.036 = 2.2925... \times 10^{-2} \)

\[
\frac{1}{\pi\alpha} \langle u_{1}|u_{3}\rangle^{2} \sim 1.0005 \sin^{2}[0.5060N_{1}] \tag{25}
\]

We note that, when \( N_{1} > 4 \), the departure from the r.h.s. of Eq. (25) (dotted line in Fig. 6) becomes significant as the transition toward the asymptotic quasiclassical Thomas-Fermi regime sets on. On the other hand, Fig. 6 displays the following chemical-potential gap transition process

\[
\mu_{3} \sim \mu_{1} \sim \Delta_{\pi}, \tag{26}
\]

where \( \Delta_{\pi} \sim \Delta_{1} \sim \Delta_{3} \sim \frac{\pi}{2} \hbar \omega_{c} \) is the common characteristic energy \( \Delta \), defined by Eq. (10), of the two eigenstates \( u_{1,3} \) about the maximum (of amplitude 1.0005 \( \pi\alpha \))
of their square scalar product $\langle u_1 | u_3 \rangle^2$, i.e. at the very peculiar quantum-dot nonlinearity $N_1 \sim N_3 \sim \pi$ related to the particular $\omega = \omega_\pi$ trap parabolicity. This value corresponds to the specific parabolic confinement $h_\omega \sim 0.14 e$ where $e = Me^2/h^2$ is the effective quantum-dot’s atomic energy unit: $\epsilon = 11.86$ meV for AsGa, thus yielding $h_\omega \sim 1.66$ meV and $\Delta_\pi \sim 2.61$ meV while $\epsilon = 27.21$ eV if the dielectric constant of the bulk material equals unity, then yielding $h_\omega \sim 3.80$ eV and therefore $\Delta_\pi \sim 5.97$ eV. According to Eq. (11), Eq. (26) yields the corresponding quantization rule for the $2E$ quantum-dot energy at $\omega \sim \omega_\pi$

$$2(E_3 - E_1) \sim 2h_\omega + \Delta_\pi. \tag{27}$$

Equations (17) and (27) show that the characteristic energy $\Delta$ which scales the electrostatic particle-particle interaction through the nonlinear differential Poisson equation (2) is in fact a true “nonlinear quantum”. Indeed, on the one hand, it is the smallest particle-particle interaction energy present in the system at vanishing nonlinearity $N \to 0$. On the other hand, the maximum of the $|u_1|u_3|^2$ transition probability between the two states is reached at resonance, i.e. either when $\Delta$ equals their nonlinear-eigenvalue chemical-potential-potential gap or when their quantum-dot energy gap is but the mere sum of the two standard “linear” radial quanta $h\omega$ and $\Delta$.

VII. CONCLUSION AND PERSPECTIVES

In the present paper, we have described the parabolic quantum dot by use of the nonlinear differential eigenproblem Eqs (12) and emphasized its relevance with respect to all existing corresponding results in the literature. This Schrödinger-Poisson (SP) differential system yields new quantum concepts such as the non-orthogonal nonlinear eigenstates $\Psi$ and their corresponding chemical-potential nonlinear eigenvalues $\mu$. In order to comply with the dimensional self-consistence between the two-dimensional electronic system and its three-dimensional electrostatics, we scaled the Poisson equation according to the characteristic energy $\Delta = \frac{1}{2}N\hbar\omega$ where $N$ is a normalized (see Eq. (10)) measure of the system nonlinearity. We showed that $\Delta$ is actually the true “nonlinear energy quantum” of the system for: i) it is the smallest additional “nonlinear” particle-particle interaction energy with respect to the standard “linear” radial harmonic quantum $h\omega$ when $N \to 0$ (see Eq. (17)); ii) it fits with that nonlinear-eigenvalue (or chemical-potential) gap between the two first zero-angular-momentum eigenstates which occurs about the maximum of their square scalar product $\langle u_1 | u_3 \rangle^2$ (see Eqs (26, 27)), i.e. about the maximum of their transition probability $\mathcal{P}$ (as a consequence of Fermi’s golden rule).

Further developments of the present work should (non exhaustively) address the two following experimental, numerical as well as theoretical topics:

1) Could the nonlinear resonance defined by Eqs (26, 27) at the very particular trap parabolicity $h\omega = h\omega_\pi$ ($= 1.66$ meV for GaAs) be observable and how? It would be a definite plus for the present model to provide an opportunity for experimental verification.

2) The $\pi\alpha$ scaling adopted in Eq. (25) seems extremely accurate. Indeed the square scalar product maximum divided by $\pi$ approaches the numerical value $1/137.036$ of the fine-structure-constant $e^2/h$ within $0.05\%$ in the latest state of our numerical simulations

$$\frac{1}{\pi} \langle u_1|u_3\rangle^2_{\text{max}} = \frac{1}{136.97}. \tag{28}$$

It seems hard to believe that Eq. (28) is but the result of a mere numerical coincidence. Rather, we wish to point out that Eq. (28) might echo Feynman’s emphasis of such a “magic number” $\frac{1}{137}$. This stunning non-relativistic property of the nonlinear-eigenstate square-scalar-product scaling will be further investigated in a future publication.

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53. 1452 (1996).
10 G. W. Bryant, Phys. Rev. Lett. 59, 1140 (1987).
11 The MathWorks, Inc. (2004), MATLAB, Version 7.0.1.24704 (R14), options = odeset('RelTol',1e-10).
12 G. Reinisch, J. de Freitas Pacheco, and P. Valiron, Phys. Rev. A 63, 042505 (2001).
13 G. Reinisch, Phys. Rev. A 70, 033613 (2004).
14 A. Szabo and N. S. Ostlund, Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory (Dover, New York, 1996).
15 R. P. Feynman and A. R. Hibbs, Quantum Mechanics and Path Integrals (McGraw-Hill Book Company, 1965).
16 G. Reinisch, Physical Review Letters 99, 120402, (2007).
17 [The numerical value $\sim 1/137$ of the fine-structure constant $\alpha = e^2/\hbar c$] ... "has been a mystery ever since it was discovered... It’s one of the greatest damn mysteries of physics: a magic number that comes to us with no understanding by man ... We know what kind of a dance to do experimentally to measure this number very accurately, but we don’t know what kind of a dance to do on a computer to make this number come out —without putting it in secretly!", in R. P. Feynman, QED: the strange theory of light and matter, University Press, (1985).