Zigzag phase transition of electrons confined within a thin annulus region

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We consider a semiclassical approach to study the possible stabilization of a zigzag phase for a system of interacting electrons confined within a thin annulus region with infinite inner/outer walls. The electrons are considered spinless and interact via the standard Coulomb interaction potential. The classical minimum energy configuration of the system due to the Coulomb repulsion between electrons is accurately determined by using the simulated annealing method. As the number of electrons increases we see the appearance and stabilization of a two-ring structure with zigzag patterns. Further increase of the number of electrons appears to eventually lead to the collapse of the two-ring zigzag structure. A simple quantum treatment of the nodal features of the free many-particle wave function shows the appearance of nodal domain patterns that are consistent with the zigzag features that were observed in the classical model.

I. INTRODUCTION

There are many models well known in the field of condensed matter physics that can be used to describe the behavior of electrons inside solids. In some instances, one thinks about electrons as being tightly bound to a particular atomic site. In many other cases, one sees the electrons as free particles that wonder from site to site. When this common situation materializes, the electrons interact strongly with both the ions in the lattice sites and with one another. A quantum treatment of this scenario leads to a very complicated many-body problem that typically cannot be solved exactly. However, ingenious theories that rely on the concept of quasiparticles reduce the difficulty of the treatment by still retaining the one-particle nature of individual electrons in the form of quasiparticles that behave somewhat like them but might have a different effective mass and distinct characteristics. This approach works very well for understanding the main features of metals and semiconductors and, generally speaking, is quite succesful on describing the properties of a large class of three-dimensuional (3D) and two-dimensional (2D) materials. Interestingly, this framework does not apply to one-dimensional (1D) systems.

In appearance, 1D electronic systems seem to be simple, but they have long been an intriguing field of study in solid state sciences and atomic physics because of their different physics from their higher-dimensional counterparts[1,2]. The main reason why 1D systems are so challenging to study by means of conventional theories is because they manifest a rich variety of exotic quantum phenomena such as charge/spin-soliton, polaron/bipolaron, bond-order wave, charge/spin-density wave, and, most noteworthy, Luttinger liquid (non-Fermi liquid) behavior[3–5]. Differently from the case of 2D and 3D systems, the quasiparticle approach for the electrons does not apply in 1D systems. In other words, one cannot treat the electrons as individual particles, but instead must consider their collective wave-like motion. The Luttinger liquid model of 1D electronic systems provides a powerful tool for understanding strongly correlated physics[6].

In principle, 1D structures allow the formation of various kinds of ordered phases. These quantum phases sometimes break the translational symmetry of lattice, charge, or spin degrees of freedom. For example, a very large number of experiments involving semiconductor quantum wires and carbon nanotubes have elucidated various features of 1D electron systems under a diverse set of situations[7–10]. Theoretically speaking, quantum fluctuations which play a very prominent role in 1D systems work to suppress any long-range ordering at a finite temperature. However, experimentally speaking, such systems are quasi-1D and not truly 1D. As a result, transverse interactions that extend beyond the limits of 1D space are usually present and play an important role in guiding the system to stabilize in an ordered state. The interplay of low-dimensionality with many other factors makes such systems even more attractive from the perspective of computational or theoretical studies with various techniques[11–15]. Therefore, understanding 1D or quasi-1D systems, the transition from 1D to quasi-1D as well as the transition from quasi-1D to 2D/3D behavior is of great interest from both a practical and a theoretical perspective[16].

A first stage for a 1D to quasi-1D transition has been predicted to involve a structural change from a 1D linear arrangement of particles to a quasi-1D zigzag configuration. While the zigzag phase of electrons is stable for a certain range of parameters, such a state eventually becomes a liquid state at higher densities. The features of the zigzag phase transition for a ring-like structure with harmonic confinement have been recently studied via quantum Monte Carlo (QMC) methods[17]. In agreement with experimental findings, the electrons confined in a 1D quantum wire by a transverse harmonic potential form a linear Wigner crystal at low densities[18,19]. On the other hand, a quasi-1D zigzag structure stabilizes at some high critical electron density[20–26]. At even higher densities, the zigzag structure is destroyed suggesting the creation of a coupled two-row structure[27]. Creation of two coupled 1D systems (quantum wires) and, more generally, creation of arrays of 1D quantum wires is a very interesting phenonenon. Understanding its features would allow one to extend the Luttinger liquid phenomenology to 2D systems when considering closely packed arrays of 1D quantum wires where each of them is being described as a Luttinger liquid.

In this work we introduce a semiclassical approach to study the zigzag phase transition in a quantum wire modeled as a system of electrons confined in a circular region with the geometry of an annulus, namely, an annular disk. To this effect, we consider an arbitrary number of electrons confined between the infinite inner wall and outer wall of the annulus. For simplicity, the electrons are considered spinless. The competition between the confinement, delocalization effects and strong Coulomb repulsion between electrons always provides a fertile ground for observation of interesting phenomena[28–30]. For the presently considered case, these factors shape the nature of the lowest energy state of the system and its geometric configuration including the possible realization of a quasi-1D state with zigzag patterns. The eventual stabilization of such a zigzag structure for specific conditions of our model is carefully studied by using the simulated annealing calculation method.

II. MODEL AND SEMICLASSICAL THEORY

The model under consideration consists of N spinless electrons confined within an annular disk region, Ω with inner radius, r_1 and outer radius, r_2 where it is assumed that $r_1 < r_2$. The center of the annulus corresponds to the origin of the chosen system of coordinates. This means that the electrons are confined within a potential well with infinite hard walls at r_1 and r_2 of the form:

$$V(r) = \begin{cases} 0 \quad ; \quad r_1 \le r \le r_2 \ , \\ +\infty \quad ; \quad \text{elsewhere} \ , \end{cases} \tag{1}$$

where r, r_1 and r_2 are 2D radial variables. Any pair of electrons i and j interact with each other via the usual repulsive Coulomb interaction potential. The quantum Hamiltonian of the system would be written as:

$$\hat{H} = -\frac{1}{2}\sum_{i=1}^{N} \nabla_i^2 + \sum_{i<j}^{N} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} + \sum_{i=i}^{N} V(r_i) \ , \tag{2}$$

where use of atomic units is implicit. As a matter of convenience, we write the inner/outer radii of the annulus as:

$$r_1 = R - \Delta \quad ; \quad r_2 = R + \Delta \ , \tag{3}$$

where R and Δ represent two new parameters that control the geometry of the domain under consideration. A schematic view of the annulus confining region is depicted in Fig. 1. With the choice of $R = 1$ and $\Delta = 1/10$, we have $r_1 = 1 - 1/10$ and $r_2 = 1 + 1/10$.

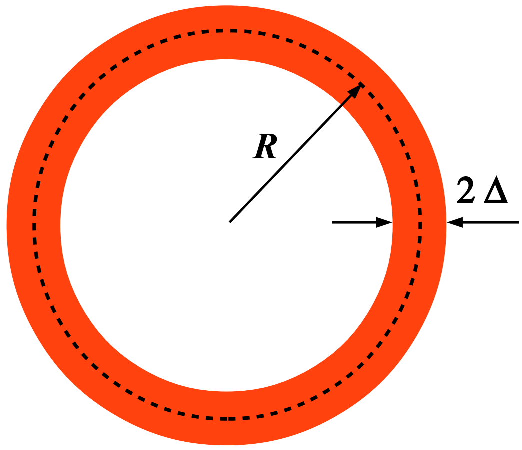

FIG. 1: Schematic view of the annulus region, Ω in which the electrons are confined. The two infinite hard walls are located at $r_1 = R - \Delta$ and $r_2 = R + \Delta$. See text for details.

A typical quantum calculation of the ground state properties of the system would imply use of sophisticated QMC techniques[31,32]. However, as a first step in our approach, we chose to adopt a semiclassical treatment. For such a framework, we look at the system from the perspective of finding the optimal electronic configuration that minimizes the total energy of Eq.(2) while discarding the first (kinetic) energy term. From this point of view, only the second term in Eq.(2), namely, the Coulomb repulsion energy is relevant. As a second step in our tretment, we will assess the magnitude of quantum effects by considering the previously discarded quantum kinetic energy term and looking at the full quantum description of a system of N non-interacting confined fermions with positions $r_1 \le r_i \le r_2$ and arbitrary angular dependence.

Within the framework of this classical treatment, there are two length scales of interest in our system. They are related to the average separation distance between: i) Charges localized in the inner radius, r_1 and ii) Charges localized in the outer radius, r_2. Let us assume that N_1 and N_2 are the number of charges at the rings with radius r_1 and r_2, respectively. The two length scales just mentioned can be defined as $r_{s1} = (2\pi r_1)/N_1$ and $r_{s2} = (2\pi r_2)/N_2$, respectively. These two length scales are, somehow, reminiscent of the Wigner-Seitz dimensionless parameter, r_s in 1D.

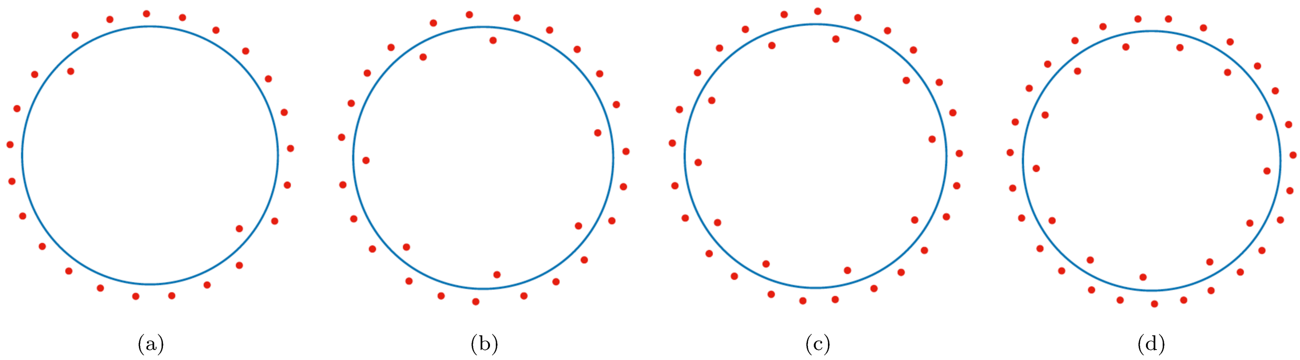

FIG. 2: Plot of the minimum electrostatic energy configurations for increasing N. The emergence of the zigzag phase is clear. Cases: (a) $N = 25$, (b) $N = 30$, (c) $N = 35$, and (d) $N = 40$. See text for details.

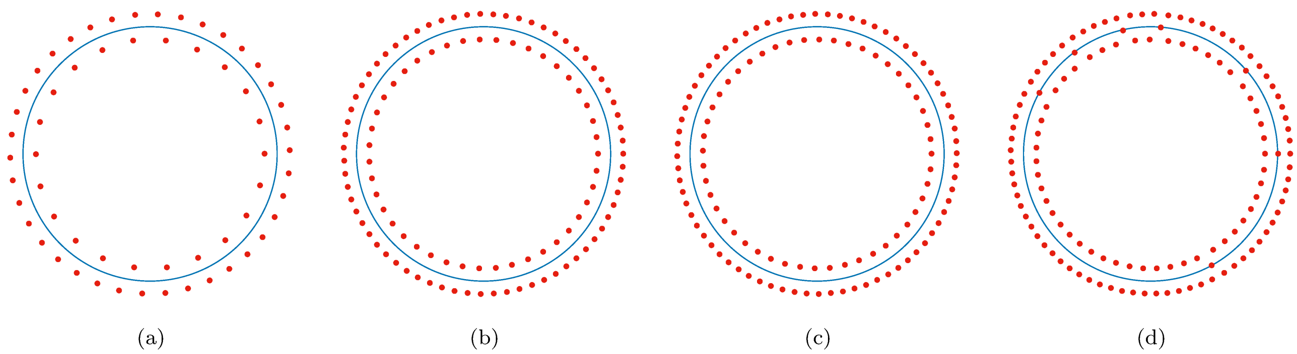

FIG. 3: Plot of the minimum electrostatic energy configurations for increasing values of N. Cases: (a) $N = 60$, (b) $N = 110$, (c) $N = 120$, and (d) $N = 130$. See text for details.

Having reached this point, the difficult task that one faces is to find the resulting geometric arrangement of electrons that leads to the lowest global energy within the constraints imposed. Therefore, one must carefully calculate the energy of the system for various given configurations and implement a minimization procedure for the total repulsion energy that results from the interaction of all the charged particles in the system. The method that we used to achieve such a goal is the simulated annealing method[33]. The simulated annealing method is one of the most successful statistical numerical methods used to date to find global energy minimums of many-particle interacting systems of the nature considered in our work. Such a method combines both the Metropolis Monte Carlo (MC) algorithm[34] and other mathematical tools to search for the global energy minimum. Various computational tools are available[35], but overall experience indicates that this method is extremely effective when used for optimization purposes. For systems on N electrons, the energy minimization process involves $2\,N$ variables since the position of each electron is represented by a 2D vector. The intricacy and duration of the calculations increases with N, but the method is fairly reliable for values of N as large as a hundred electrons.

The emergent transition from a single-row to a double-row distribution (string zigzag transition) does happen at around and above $N = 25$ as can be appreciated by looking at Fig 2 where we show the most stable configurations of electrons for increasing values of number $N = 25, 30, 35$ and 40. One notices that the zigzag structure fully unfolds at $N = 40$. The range of N shown in Fig 2 illustrates well the first occurrence of the transition from a single-row to a double-row as N increases.

Pertinent results for $N = 60$, 110, 120 and 130 electrons are shown in Fig 3. A zigzag configuration is clearly identifiable for these specific systems. One also notes that, as the number of electrons continues to increase, the average distance between the particles, r_{s1} and r_{s2} gradually diminishes up to a point where it becomes favorable to promote the new particles not at the two rings, but in the central ring at R (see case of $N = 130$).

The distribution of 7 electrons in the third (middle) row shown in Fig 3(d) for the case of a total of $N = 130$ particles is asymmetric. Since the number of metastable states increase exponentially with size it becomes harder and harder to find accurately the global energy mininum. While the emergence of a third (middle) row is certainly not a spurious effect, it is most likely that this precise asymmetric configuration belongs to a metastable state that is very close in energy to the global minimum energy. However, the key point to reason is that the onset of a third row nevertheless occurs. The exact energy of the real (likely symmetric) configuration is not of vital importance in this study. This means that the zigzag state becomes unstable and eventually ends at some critical number N. Systems with N larger than this critical value (namely, systems with increased density values) eventually would collapse into structures that are different from the two-ring zigzag state seen for values of N such as $N = 60$ or $N = 110$ as an example. At this juncture, we point out that it is not easy to compare our classical results with quantum ones. However, the way that we understand this problem, the rupture of the zigzag phase will eventually occur in the form of the appearance of an intermediate ring. This is the precise situation that is encountered in the quantum case, too[17].

At a sufficiently large number of electrons ($N \propto 120$ in the classical calculation), rather than viewing the structure of the electron distribution as zigzag, one can view it as two discrete chains of electrons, where the distance between the electrons within each chain is already quite small compared to the distance between the chains. In this regard, one may wonder about the energy of the potential barrier that must be overcome in order for one row of a zigzag structure to move relative to another or whether is it possible to independently control the conductance of one of the two rows[36,37]. The latter question regarding control of the conductance departs too much from the the orginal aims of this work and it is difficult to answer. As far as the prior question, we point out that, at some point, one can even retrieve an expression for the total energy for the system with two rows or chains. The total energy for N particles forming a regular polygon of radius r is given by:

$$E_N(r) = \frac{k_e}{2\,r} \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \frac{1}{\sin \frac{\pi}{N}(|i-j|)} = \frac{k_e N}{4\,r} \sum_{k=1}^{N-1} \frac{1}{\sin \frac{\pi}{N} k} \tag{4}$$

where $k_e = e^2/(4\pi\varepsilon_0\varepsilon_r)$. For two concentric regular rings with radii, $R_1 < R_2$ and occupation numbers, N_1 and N_2 (where $N_1 + N_2 = N$), respectively, we encounter the average energy[38]:

$$\begin{aligned} E_{\rm mean}(N_1, N_2, R_1, R_2) \,/\, k_e \;=\; & \frac{N_1}{4R_1} \sum_{k=1}^{N_1-1} \frac{1}{\sin \frac{\pi}{N_1} k} \\ + \frac{N_2}{4R_2} \sum_{k=1}^{N_2-1} \frac{1}{\sin \frac{\pi}{N_2} k} \;+\; & \frac{2}{\pi}\, N_1\, N_2\, \frac{K(R_1/R_2)}{R_2}\,, \end{aligned} \tag{5}$$

where K is the complete elliptic integral of first kind. One has to bear in mind that R_1 and R_2 can be considered as known in our context and consider N_1, N_2 as the only variables to optimize (subject to the condition that $N_1 + N_2 = N$ is kept fixed). The last term in the previous expression is obtained by averaging the relative angle position. This expression would be valid for N around and not much greater that $N = 120$ (where structures with two chains are present).

The consideration of zigzag structures of electrons is certainly not novel, from the classical point of view. It is also known that presence of a harmonic oscillator (HO) confinement plus the interaction between charges makes the system more realistic as well as more challenging to handle. In a recent work, Piacente et al.[11] carried out elaborate Monte Carlo studies of a quasi-1D system of charged particles interacting through a Yukawa-type screened Coulomb potential with a controllable screening length. In that study, the ground-state energy was calculated and, depending on the density and the screening length, the system crystallizes in a number of chains. The combination of the interaction among particles and the confining potential displays a rich structural phase diagram as a function of the density (or the confining potential) at both zero and nonzero temperature. Our system has a different confinement potential (thin annulus with hard walls) and has a circular symmetry. Despite its simplicity, it allows one to observe the onset of a zigzag transition for certain values of the parameters. Thus, similar qualitative parallels can be drawn regarding our final results and those by Piacente et al.[11] despite the fact that the latter work considers a more realistic system that lacks the circular symmetry of ours.

III. QUANTUM APPROACH

We now go beyond the earlier semiclassical treatment and provide an estimate of the impact that the quantum kinetic energy term has on the properties of the system. The quantum system of electrons confined within the annulus region considered in our work can be viewed as the quantum counterpart of the so-called classical billiard. The classical billiard is a dynamical system consisting of a point particle moving freely in an enclosure, alternating between motion along a straight line and elastic reflections off the boundary[39,40]. This sequence of specular reflections is captured by the billiard map, which completely describes the motion of the particle.

Over the last two decades, the quantum analogues of the classical billiard systems, namely, the quantum billiards, have been experimentally realized in gated, mesoscopic GaAs tables[41] or microwave cavities[42]. It has been found that eigenfunctions of these planar billiards organize themselves into regions, or domains, with positive and negative signs, often in remarkably complicated geometric shapes. Formally, such nodal domains may be defined as the maximally connected regions wherein the wave function does not change sign. Experimentally, nodal domains have also been the focus of much attention[43–45].

For the 2D annular disk confining region of our model, one writes the stationary Schrödinger's equation of the particle in 2D polar coordinates as:

$$-\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial r^2} \,+\, \frac{1}{r}\frac{\partial}{\partial r} \,+\, \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2}\right)\psi(r,\theta) \;=\; E\,\psi(r,\theta)\;, \tag{6}$$

where r is the 2D radial distance, θ is the azimuth (polar) angle, $\hbar$ is Planck's reduced constant and μ is the (reduced) masss of the particle. Utilizing the usual separation of variables for the wave function, $\psi(r,\theta) = R(r)\,\Theta(\theta)$, the angular part has a solution of the form:

$$\Theta_m(\theta) \,=\, \frac{1}{\sqrt{2\,\pi}} e^{i\,m\,\theta} \quad ; \quad m = 0, \pm 1, \pm 2, \ldots \;, \tag{7}$$

where $\theta \in [0, 2\pi)$. With the change of variable to $z = k\,r$ where $k = \sqrt{2\mu E/\hbar^2}$, the differential equation for the radial part of the wave function becomes:

$$\frac{d^2 R(z)}{dz^2} + \frac{1}{z}\frac{dR(z)}{dz} + \left(1 - \frac{m^2}{z^2}\right) R(z) \,=\, 0 \;. \tag{8}$$

The solution of this differential equation is given by:

$$R(r) \,=\, \alpha\, J_m(k\,r) + \beta\, Y_m(k\,r) \;, \tag{9}$$

where $J_m(x)$ ($Y_m(x)$) is the m-th order Bessel function of the first (second) kind and α, β are arbitrary constants. Note that $Y_m(x=0)$ is divergent. However, the origin is not part of the annulus domain. Therefore, the most general solution is, indeed, the expression in Eq.(9).

The Dirichlet boundary conditions require that the wave funtion be zero at both locations $r = r_1$ and $r = r_2$ regardless of the angular dependence. One can write the resulting equations for the unknown quantities α and β in matrix form. Since we are looking for nonzero solutions for α and β, we must require that the determinant of the coefficient matrix be zero[46]. This means that the eigenenergies (the values of k) must satisfy the following equation:

$$J_m(k\,r_1) Y_m(k\,r_2) \,-\, J_m(k\,r_2) Y_m(k\,r_1) \,=\, 0, \tag{10}$$

where $k_{m,n_r} = \sqrt{2\,\mu\,E_{m,n_r}/\hbar^2}$ would represent the roots (zeros) of the above equation. Hence, the energy spectrum must be retrieved by numerically solving for the roots of the expression in Eq.(10). Note that the value of k_{m,n_r} cannot be zero. The first positive root that solves Eq.(10) is labeled $n_r = 1$, the second one is labeled $n_r = 2$ and so on. Furthermore, one must remember that all nonzero values of m are 2-fold degenerate.

The Dirichlet boundary conditions at $r = r_1$ and $r = r_2$ lead to a radial wave function of the kind:

$$R_{m,n_r}(r) \,=\, N\left[J_m(k_{m,n_r} r) Y_m(k_{m,n_r} r_1) \,-\, J_m(k_{m,n_r} r_1) Y_m(k_{m,n_r} r)\right] \;, \tag{11}$$

where $r \in [r_1, r_2]$ and N is an irrelevant normalization constant. Since $\psi_{m,n_r}(r,\theta)$ and $\psi_{-m,n_r}(r,\theta)$ have the same energy, one can form linear combinations, for instance, $R_{m,n_r}(r)\,\cos(m\,\theta)$ that represent real wave functions. We can plot them for increasing values of k_{m,n_r} (energy). In particular, the many-particle wave function for a given range of values of the number of fermions, N is displayed in Fig 4. The fermionic case requires all energy eigenvalues, E_{m,n_r} to be sorted in increasing order. This energy spectrum involves, of course, a discontinuous "staircase" function for the total number of particles at zero temperature of the form:

$$N \,=\, \sum_{m,n_r} \Theta(E_F - E_{m,n_r}) \;, \tag{12}$$

as well as the total energy:

$$U_0 \,=\, \sum_{m,n_r} E_{m,n_r}\, \Theta(E_F - E_{m,n_r}) \;. \tag{13}$$

The procedure previously outlined has to be performed numerically. Assuming the Fermi energy E_F to be the n-th sorted eigenenergy E_{m,n_r}, we count the number of contributions including the degeneracy, g_{m,n_r} associated with any given $\{m, n_r\}$ state. In other words, we calculate $N = \sum_k g_k$ where, in a short-hand notation, $k \equiv k_{m,n_r}$. In this fashion, we retrieve the number of particles N as a function of E_F.

The shape of the container of the free electron gas is not relevant in the thermodynamic limit. This amounts to having a smoothed expression for the Fermi energy as a function N while N increases asymptotically. Weyl's law[47,48] is the mechanism that guarantees the earlier statement provided that the system is *integrable* in the language of quantum billiards. Mathematically speaking, Weyl's law states that the typical staircase of the internal energy that appears for any finite system of fermions is smoothed out in a way that does not depend on the shape of the domain, Ω that contains the particles when the number of particles is large (in the thermodynamic limit). In other words, the only thing that matters is the volume that is occupied by the particles. The shape, be it a parallelogram or a sphere, is not relevant. Otherwise Weyl's law in its current form has to be modified. For the particular case of a 2D shape of area A and perimeter P, the number of normal mode wave numbers in the range $(k, k + dk)$ is given by:

$$dN(k) = \left(\frac{A}{2\pi} k - \frac{P}{4\pi}\right) dk \;. \tag{14}$$

FIG. 4: Plot of the many-particle wave function of the sorted spectrum of the annulus as we increase the number of fermions, N. We observed that, for the quantum counterpart of the electrostatic classic cases, several domains appear everywhere the wave function changes its sign. The first instance occurs at $N = 58$ and finishes at $N = 158$. Within this range, the zigzag structure happens starting from the radial quantum number, $n_r = 2$. It ends abruptly beginning from $N = 159$ where three "stripes" begin to appear. See text for details.

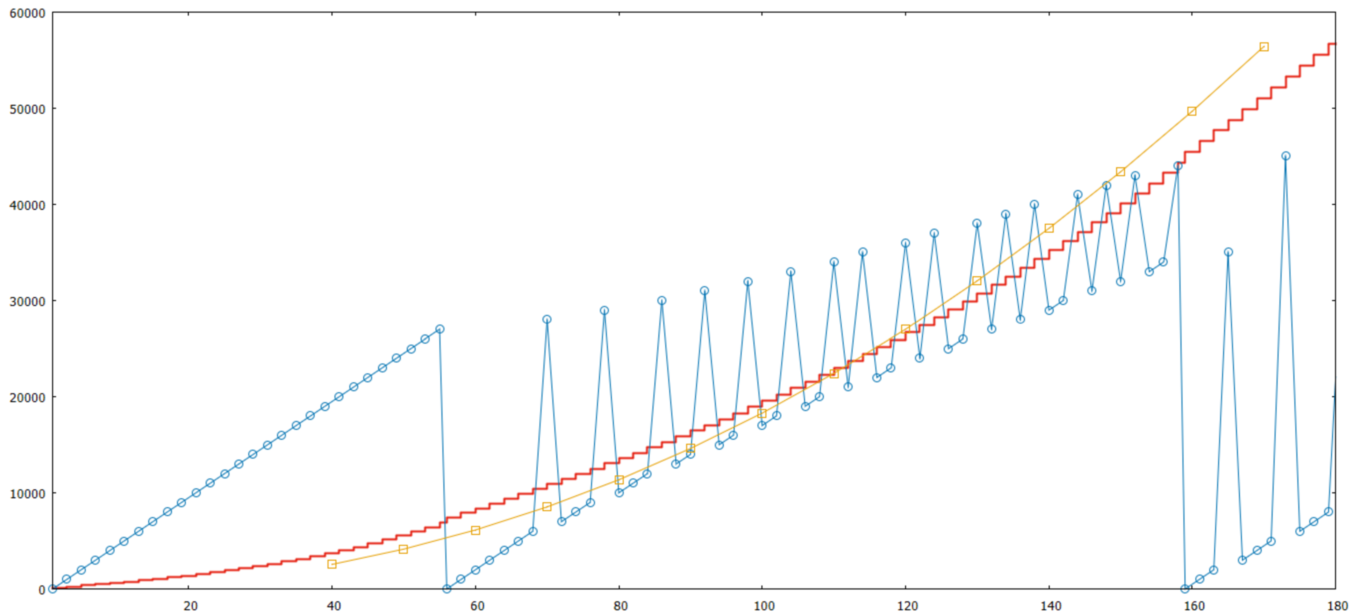

FIG. 5: Total energy, U_0 at $T = 0$ K (not the Fermi energy) vs N (red staircase) for the system of free fermions confined inside the annulus with parameter values, $R = 1$ and $2\,\Delta = 2/10 = 1/5$. The angular momentum of the last added particle (enhanced 1000 times) is also shown (empty circles). The total electrostatic energy (enhanced 3 times) is represented by the intermediate line (squares). See text for details.

Upon integration, this gives:

$$N(k) = \frac{A}{4\pi}k^2 - \frac{P}{4\pi}k \ , \tag{15}$$

or, in the present context:

$$N(E) = \frac{A}{4\pi}\left(\frac{2\mu}{\hbar^2}E\right) - \frac{P}{4\pi}\sqrt{\frac{2\mu}{\hbar^2}E} \ . \tag{16}$$

Hence, the Weyl-like result in Eq.(16) represents an approximation to a smoothed out version of the numerical results.

At this stage, one might raise the question of how does our approach to the problem justifies the treatment of the system as free particles confined in an annular disk region? The answer to this question is that, indeed, this is the simplest approach that retrieves a non-trivial spectrum and, intuitively, can account for the existence of a zigzag phase of the electrons. For instance, we have in Fig. 4 an example of how the eigenfunctions look like. The definitions of sectors or *domains* limited by the nodes of the many-particle wave function constitutes an approximation to the problem even without including the Coulomb interaction.

In the quantum study we consider systems with "filled" energy shells (so that number of particles that occupy a given degenerate energy level is the same as number of degenerate states associated with that level). For this choice, the electrons occupy all the quantum states starting from the lowest to the highest energy. The degeneracy is the one that defines the number counting. The total number of particles is defined as $N = \sum_{m,n_r} g_{m,n_r}$ where energy states with $m \neq 0$ are two-fold degenerate while those with $m = 0$ are not degenerate (degeneracy 1). The first few states are filled starting from $(m = 0, n_r = 1)$ (degeneracy 1), $(m = \pm 1, n_r = 1)$ (degeneracy 2) and so on, but then, at some point, comes a state of the form $(m = 0, n_r = 2)$ (degeneracy 1). It turns out that, when we go from one "filled" energy shell to another, the number N grows mostly in steps of 2 (since there are more $m \neq 0$ states than $m = 0$ states) and less times by one (when states with $m = 0$ values are encountered). Based on this approach, the next system that comes after $N = 56$ is that with $N = 58$ particles. The system with $N = 58$ particles is the first instance displaying a double-row electron structure.

It can be seen from Fig. 5 that even the behavior of the angular momentum as we add particles to the system provides a plausible explanation for the occurrence of a zigzag phase transition. Fig. 5 displays three quantities: i) The angular momentum of the last added particle (empty circles), enhanced 1000 times; ii) The total energy of the non-interacting fermions (red staircase) at zero temperature; and iii) The equilibrium energy for the classical case (squares), enhanced 3 times. These three quantities depend on the number of particles, N. Notice that, for the quantum case under consideration, it takes into account the degeneracy. The region between two consecutive zero values of the angular momentum provides the region where the zigzag phase can occur as displayed in Fig. 4. Thus, a non-interacting approach to the system using confined fermions can also account in a similar way as the purely classical, electrostatic one. Incidentally, the energies in the quantum case are higher.

IV. DISCUSSION AND CONCLUSIONS

It is important to discuss the role of the confinement potential in the overall picture. The model under consideration exploits a hard wall potential in a thin annulus region, but in experimental studies of quasi-1D quantum wires confinement can be much softer, approaching to a harmonic one as noticed in various works[49,50]. Overall, the nature of the confinement influences very much the degree of localization. This means that replacing the present confinement with a HO confinement, for the sake of illustration, will indeed change the structure of the stable configurations of the system because we now have a competition between confinement and repulsion. If we scale the whole Hamiltonian in terms of e^2/R, we are left only with a free parameter depending on the angular frequency, ω_0 for the HO parabolic confinement potential. Previous calculations have shown that the ensuing electron distribution strongly depends on the value of the frequency ω_0. The effect of a frequency that is sufficiently high is to disguise the onset of any zigzag transition. This means that a HO confinement does not help in enhancing the formation of a zigzag phase in the classical case. The quantum case is different and far more difficult to analyze.

The interplay of various forms of confinement and other parameters in the system (such as electron density, interaction, spin, externally applied magnetic field, etc.) leads to interesting experimental findings. For example, Hew et al.[51] have studied the low-temperature transport properties of 1D quantum wires as the confinement strength and the carrier density are varied. Their results show the beginnings of the formation of an electron lattice in an interacting quasi-1D quantum wire. Kumar et al.[52] investigated electron transport in a quasi-1D electron gas as a function of the confinement potential. It was noticed that, at a particular potential configuration and electron concentration, the ground state of a 1D quantum wire splits into two rows to form an incipient Wigner lattice. In addition, it was found that application of a transverse magnetic field can transform a double-row electron configuration into a single row. This means that an in-plane magnetic field can tune both the degree of the confinement and the nature of the energy spectrum. Similarlly, Kumar et al.[53] studied the electron transport in quasi-1D quantum wires in GaAs/AlGaAs heterostructures obtained using an asymmetric confinement potential. Their results show how the behavior of the system can be affected by the inhomogeneity in background potential and they observed the formation of double rows of electrons.

In this work, we studied the geometric arrangement of a system of N electrons confined in a 2D annular region with infinite hard hard walls at $r_1 = R - \Delta$ and $r_2 = R + \Delta$. For simplicity, it is assumed the electrons are spinless. The interplay bettwen N, R, Δ and the Coulomb repulsion between electrons determines the lowest energy arrangement of the system. We choose specific values of R and Δ and aimed to obtain the lowest energy configuration of the system as the number, N of electrons is varied. As a first step, we adopt a semiclasical approach and look at determining what geometric configuration of electrons has the lowest energy that minimizes the total Coulomb repulsion energy of the system. The idea is to see whether a two-ring zigzag structure emerges as the global energy mininum for the system under consideration.

Finding the global energy minumn for an interacting system of this nature is a very challenging problem. Specialized numerical methods must be used and utmost care must be exercised since there are instances in which the system may get "stuck" in a local energy mininum. We use the simulated annealing method to solve this many-particle minimization problem as accurately as possible. The method is effective and efficient timewise for systems as large as of the order of $100 - 200$ electrons. The results indicate the stabilization of a two-ring structure with zigzag patterns for a wide range of values of N considered in this work. However, as the number of electrons grows larger, one envisions the collapse of the two-ring zigzag structure to a more extended geometric arrangement. This implies that there is a range of system sizes, namely, density values where the zigzag structure emerges. Other non-zigzag structures may eventually stabilize outside this range.

A complementary approach would introduce quantum features in the model by considering an appropriate many-particle wave function and take into account the quantum kinetic energy of the system of non-interacting fermions, namely, the ensemble of electrons trapped between the walls of the 2D annular confining domain. In this case, we study the emergent nodal features since they indicate inherent patterns for this system that can be viewed as a quantum billiard-like setup. The nodal features of the many-particle wave function indicate a nodal domain pattern that is consistent with zigzag features observed at those particular values of N that we considered.

Along these lines, it is somehow surprising to see that two different approaches give qualitatitely similar results. In the classical case, it is not difficult to understand intuitively that the bare Coulomb repulsion is responsile for the appearance of the two-row zigzag structure within the constraint of the hard-wall confinement. With regard to the (simplified) quantum model where no interaction is considered, we believe that the combined effect of the specific hard-wall annular confinement in conjunction with the Fermi statistics is the key actor responsible for the observed "localization" of the particles. Therefore, it is not inconceivable to speculate that it is possible that a structural phase transition from a 1D chain to a zigzag structure can occur for electrons in a very strong hard-wall confinement inside a thin annulus region even in the absence of interaction (or when the interaction is quite weak). This state might also bear resemblance to a double-row structure or (for the case of an infinitely thin annulus with hard-walls) to a "string-zigzag" transition as discussed in a recent work by Mahmoodian et al.[16].

Obviously the quantum mechanical treatment is oversimplified since it does not include electron interaction and correlation effects in a broader context. A more realistic quantum treatment along these lines can be done via QMC and/or density functional theory (DFT) methods. For example, accurate DFT numerical studies by Yakimenko et al.[15] show how one can investigate rather intricate systems in structures consisting of quantum wires and quantum point contacts (QPCs) that have been realized in GaAs/AlGaAs heterostructures. This paper studies the electron transport through a wide top-gated QPC in a low-density regime based on DFT methods. It shows how the electron–electron interaction and shallow confinement affect electron conduction and spin polarization. Earlier work[50] on similar systems also showed subtle effects that relate the occurrence of local magnetization and the effects of electron localization in different models of QPCs. In the case of soft confinement potentials the degree of electron localization is weak. However, when a strong confinement potential is achieved, electron localization is favored in the relatively low density regime. In such cases one may create a variety of electron configurations ranging from a single localized electron to structures with multiple rows and Wigner lattices.

To summarize, the stabilization of a zigzag structure for specific conditions is carefully studied by using the simulated annealing calculation method. We have presented two complementary ways of describing the onset of the zigzag state with results that seem to be quite robust for the range of N considered in this work The original work that described the existence of a zigzag phase[17] considered a HO confinement plus the Coulomb interaction. The specific setting makes the scale of energies and the number of particles where the phase appears dependent on the nature of the confinement potential. In our approach, we cover an extreme localization scenario (classical case) and a non-interacting one (quantum case, fermions). Both are able to roughly predict the same number of particles where the zigzag phase does occur. This alternative description of the system departs from the one originally studied[17], but that does not affect the findings of the present work. After all, our results consider and support the existence of such zigzag phase, albeit with different energy scales and a different type of confinement potential.

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