"Ground state energy of 2-D charged particles clusters: A study by Quantum Monte Carlo method"

N. L. Moreira, L. Cândido and J. N. Teixeira Rabelo
Instituto de Física, Universidade Federal de Goiás, 74.001-970, Goiânia (GO), Brazil
e-mail: nilton.luis@bol.com.br / jrabelo@fis.ufg.br

We have studied the ground state energy of 2-D few charged-spinless-particles confined by a parabolic potential, using quantum Monte Carlo method. This is a model to treat systems like semiconductors quantum dots.

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I. INTRODUCTION

The technological advance in the preparation and in the fabrication of microstructures yields nowdays to confine electrons and atoms in restricted regions. The main experimental progress in this area are the semiconductor quantum dots [1] and the laser trapps of cold atoms [2]. The semiconductor quantum dots constitute a quasi ideal system for the study of the physical properties of a two-dimensional system of strongly interacting electrons, laterally confined by an external potential. From the theoretical point of view, the computing simulation [3] has achieved the greatest success inusmuch as the analytical approximated methods [4, 1] has encountered dificulties, since both the many body effects and the indivicual behavior of each electron have indeed a crucial role in these systems, and the major dificulty in the theoretical methods is due to the fact that the electrons in the quantum dots are confine in a very small area and hence they can not be treated as part of a continuous distribution of charges. These systems constituted of a finite number of electrons, confined in small regions in semiconductor structures are known as quantum dots and more recently also as artificial atoms.

The Schrödinger equation is the basis for the microscopic description of materials in the various states of aggregation. But, its analytical solution is possible only for some very simple models. Because of this, the development of numerical methods for the solution of this equation is of great interest. Several methods have been developed in recent years and among them one is been specially successful and has been named the Diffusion Monte-Carlo Method (DMC). This method has been showing to be adequate to describe the ground state of various systems.

In this work, we want to present a calculation of the ground state energy of various two-dimensional clusters of charged spinless particles using a Diffusion MOnte Carlo (DMC). These objects are of great interest because they manifest some atomic-like properties.

We organize our paper as follows. In the section II we present the model for the quantum dots and we present the Quantum Monte Carlo method. The section III contains our results and the last section IV contains our conclusions.

II. THE MODEL AND METHOD

The usual model for a disk-shaped vertical quantum dot is a 2-dimensional system of N electrons moving in the $z = 0$ plane, confined by a parabolic lateral confining potential $V_{con}(\mathbf{r})$[5]. The Hamiltonian is given by:

$$H = \sum_{i=1}^{N} \frac{-\hbar^2}{2m_e}\nabla_i^2 + \sum_{i=1}^{N} V_{con}(\vec{r}_i) + \frac{e^2}{\epsilon}\sum_{i<j}^{N}\frac{1}{|\vec{r}_i - \vec{r}_j|} \quad (1)$$

In Eq. 1, m_e is the electron mass and ϵ is the dielectric constant. We have used atomic units defined by: $\hbar = e^2/\epsilon = m_e = 1$.

1. Monte Carlo Integration

In the DMC for some multidimensional integral we have[6]:

$$I = \int_{-\infty}^{\infty}\left(\prod_{j=0}^{N-1} dx_j\right) f(x_0, \cdots, x_{N-1})\, P(x_0, \cdots, x_{N-1})$$

$$\int_{-\infty}^{\infty}\left(\prod_{j=0}^{N-1} dx_j\right) P(x_0, \cdots, x_{N-1}) = 1.$$

According with the last equation the integral of the propability $P(n) = 1$ and the estimate of the first integral is I':

$$I' = \frac{1}{\check{N}}\sum_{i=1}^{\check{N}} f\left(x_0^{(i)}, \cdots, x_{N-1}^{(i)}\right),$$

2. Diffusion Monte Carlo method

The basis of Diffusion Monte Carlo method (DMC) is the Schrödinger equation in imaginary time. One can think of this equation as a diffusion equation (with diffusion constant $D = \hbar^2/2m$) with an additional

branching term, given by the potential energy[7]. This equation can be written as

$$-\frac{\partial\phi\left(x,\tau\right)}{\partial\tau}=\left(H-E_{T}\right)\phi\left(x,\tau\right) \tag{2}$$

If $\phi\left(x,0\right)$ is expanded in the eigenvectors of the H, with eigenvalues E_1, E_2, ..., E_k, then ϕ evolve in time as:

$$\phi\left(x,\tau\right)=C_{0}\Phi_{0}e^{-\left(E_{0}-E_{T}\right)\tau}+C_{1}\Phi_{1}e^{-\left(E_{1}-E_{T}\right)\tau}+\cdots \tag{3}$$

$$\phi\left(x,\infty\right)\approx C_{0}\Phi_{0}e^{-\left(E_{0}-E_{T}\right)\tau}$$

We seek a quantum mechanical operator with the following projection properties:

$$\phi\left(x_{2},\tau_{2}\right)=\int G(x_{2},\tau_{2};x,\tau_{1})\phi\left(x,\tau_{1}\right)dx \tag{4}$$

Here $G(y,\tau_2;x,\tau_1)$ is the Green's function which projects an initial state$|\phi,\tau_1\rangle$ forward in imaginary time to $|\phi,\tau_2\rangle$.

$$\left|\phi,\tau_{2}\right\rangle=G(\tau_{2};\tau_{1})\left|\phi,\tau_{1}\right\rangle \tag{5}$$

$$G(x_{2};x_{1},\delta\tau)=\left\langle x_{2}\right|e^{-H\delta\tau}\left|x_{1}\right\rangle \tag{6}$$

For small values of $\delta\tau$ we may use the commutator expansion, using $H=K+V$:

$$e^{-H\delta\tau}\approx e^{-\frac{1}{2}V\delta\tau}e^{-K\delta\tau}e^{-\frac{1}{2}V\delta\tau}\equiv G_{dif}G_{tax} \tag{7}$$

$$G-G_{dif}G_{tax}=\frac{1}{2}\left[K,V\right]\left(\delta\tau\right)^{2}+O(\delta\tau)^{3}$$

$$G(x_{2};x_{1},\delta\tau)=\left\langle x_{2}\right|e^{-\frac{1}{2}V'\delta\tau}e^{-K\delta\tau}e^{-\frac{1}{2}V'\delta\tau}\left|x_{1}\right\rangle \tag{8}$$

$$\int dx_{4}\int dx_{3}\left\langle x_{2}\right|e^{-\frac{1}{2}V'\delta\tau}\left|x_{4}\right\rangle\left\langle x_{4}\right|e^{-K\delta\tau}\left|x_{3}\right\rangle\times \left\langle x_{3}\right|e^{-\frac{1}{2}V'\delta\tau}\left|x_{1}\right\rangle. \tag{9}$$

The equation 9 in the momentum representation where $K=DP^2$, $D=\hbar^2/2m$:

$$\int dP\left\langle x_{2}\right|P\rangle e^{-DP^{2}\delta\tau}\left\langle P\right|x_{1}\rangle\, e^{-\left[V'(x_{2})+V'(x_{1})\right]\frac{\delta\tau}{2}}$$

$$\int dPe^{iP\cdot x_{2}}e^{-DP^{2}\delta\tau}e^{iP\cdot x_{1}}e^{-\left[V'(x_{2})+V'(x_{1})\right]\frac{\delta\tau}{2}}$$

$$G(x_{2};x_{1},\delta\tau)\approx e^{-\frac{(x_{2}-x_{1})^{2}}{4D\delta\tau}}e^{-\left[V'(x_{2})+V'(x_{1})\right]\frac{\delta\tau}{2}}$$

$$\phi\left(x_{2},\tau_{2}\right)=\int e^{-\frac{(x_{2}-x_{1})^{2}}{4D\delta\tau}}e^{-\left[V'(x_{2})+V'(x_{1})\right]\frac{\delta\tau}{2}}\phi\left(x_{1},\tau_{1}\right)dx \tag{10}$$

3. *Importance Sampling*

To improve the simulation of Eq.2 we introduce the importance sampling procedure in order to avoid divergences caused by branching rate constant (E_T-V). In this procedure, one constructs an analytical trial function,Ψ, based on any available knowledge of Φ_0. Typically, Ψ is generated from standard methods, such as Hartree-Fock, etc[8]. The trial function is then used to produce the distribution $f(x,\tau)\equiv\phi(x,\tau)\Psi(x)$ rather than $\phi(x,\tau)$. If we multiply the Eq. 2 by Ψ and rewrite in terms of $f(x,\tau)$, we find,

$$\begin{aligned}-\frac{\partial f\left(x,\tau\right)}{\partial\tau} &= D\nabla^{2}f\left(x,\tau\right)-D\nabla\bullet\left(f\left(x,\tau\right)\mathbf{F_{Q}}(\mathbf{x})\right)\\ &+\ \left(E_{T}-E_{L}\right)f\left(x,\tau\right)\end{aligned} \tag{11}$$

where $E_L\equiv H\Psi/\Psi$ is the local energy, and $\mathbf{F_Q}\equiv\mathbf{2\nabla\Psi/\Psi}$ is the quantum force vector. The importance sampling changes the Green's function. The branching part can be obtained by replacing V with E_L and the diffusion part, the "kinetic energy" operator takes the form

$$K'=-D\nabla^{2}+D(\nabla\bullet\mathbf{F_{Q}})+\mathbf{D}(\mathbf{F_{Q}}\bullet\nabla). \tag{12}$$

III. RESULTS

We have used in this simulation a Variational Monte Carlo program in order to optimize the trial wave function parameters. The trial wave function is constituted by a product of two gaussian and a Pade's factor in order to take into account the electron-electron correlation as follow:

$$\Psi_{T}=e^{-Z(\sum_{i=1}^{N}r_{i}^{2}+\sum_{j=1}^{N}r_{j}^{2})}e^{\sum_{i=1}^{N}\sum_{j>i}^{N}\frac{\beta r_{ij}}{1+\alpha r_{ij}}}$$

where Z, α and β are variational parameters. A Diffusion Monte Carlo was used for obtain the ground state energy of the quantum dot.

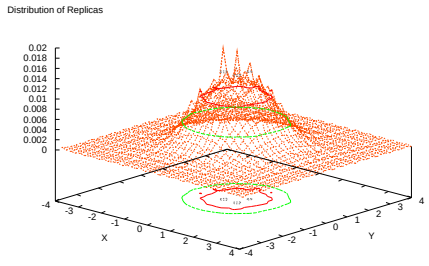

FIG. 1: *Distribution of walkers for 3 particles*

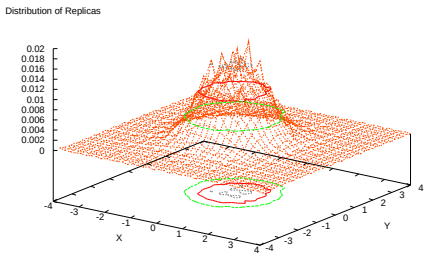

FIG. 2: *Distribution of walkers for 4 particles*

The figures 1 and 2 show the distribution of replicas for 3 and 4 particles respectively. Its localization are displayed by level surfaces. The figure 3 show the fast convergence of the trial energy for 3 particles and in the figure 4 we present the ground state energy for $2 \leq N \leq 6$. The bigger cross shows the results of ref.[5] for particles with spin, and the small cross show our results.

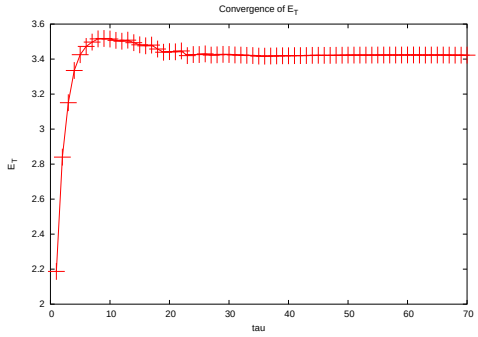

FIG. 3: *The fast convergence of DMC for 3 particles*

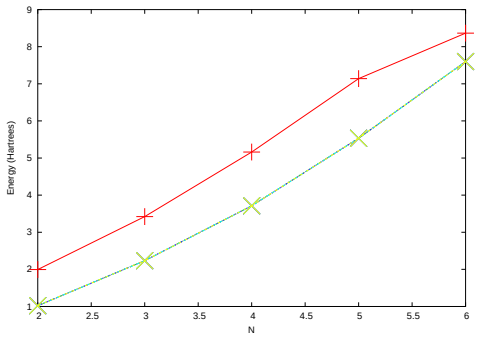

FIG. 4: *Ground state energy comparacion with results of ref [5] (bigger cross)*

IV. CONCLUSIONS

We presented a still incomplete study of the ground state energy of 2-D charged particles clusters using the Quantum Monte Carlo Method. Comparison of the values for energies are complicated by the fact that various authors use different values for the parameters. We note, however, that the behavior of the curves are in a good agreement.

Acknowledgements

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