Journal of Physics: Conference Series **563** (2014) 012007 doi:10.1088/1742-6596/563/1/012007

Ground state configurations of charged particles in a disk at zero temperature

M. Cerkaski[1] **and R.G.Nazmitdinov** [2,3]

[1] Henryk Niewodniczanski Institute of Nuclear Physics, Department of Theoretical Physics, Krakow, Poland
[2] Departament de Física, Universitat de les Illes Balears, 07122 Palma de Mallorca, Spain
[3] BLTP, Joint Institute for Nuclear Research, 141980 Dubna, Russia

E-mail: Marcin.Cerkaski@ifj.edu.pl

Abstract. We discuss a novel theoretical approach which explains the self-organization of charged particles in a disk geometry. It allows to calculate readily equilibrium configurations for $n \leq 400$ with a remarkable accuracy, when compared with the molecular dynamics calculations.

1. Introduction

There is an enormous interest in mesoscopic systems consisting of a finite number of interacting particles in confined geometry [1, 2]. Progress in a modern technology allows to study various phenomena on the same scale, from Bose condensate with thousand atoms to quantum dots with a few electrons, providing a rich information about correlation effects in such systems. Nowadays many ideas and concepts introduced, for example, in condensed matter are realized and analysed with a high accuracy. In particular, long ago Wigner predicted for electrons interacting by means of the Coulomb forces in a three-dimensional space the onset of crystallization at low enough densities and temperatures [3]. At these conditions the potential energy dominates over the kinetic energy and defines the equilibrium configurations of electron systems. Indeed, signatures of the Wigner crystallization were observed in two-dimensional (2D) distributions of electrons on the surface of liquid helium [4].

Nowadays the question how a finite number of charged particles arrange themselves in a restricted planar geometry attracts many researches. J.J. Thompson was among first who suggested an instructive solution for interacting electrons, reducing the 3D harmonic oscillator confinement potential to a circular (2D) harmonic oscilator [5]. He developed an analytical approach which enables to one to trace a self-organization of a small number of electrons in a family of rings (shells) with specific numbers of electrons. Although the number of particles in outer and inner rings are changing as a function of the total number of electrons, each shell is characterised by a certain discrete symmetry. Namely, N point charges located on the ring create equidistant nodes on the ring, with the angle $\alpha = 2\pi/N$. Similar shell pattern have been found much later by means of Monte–Carlo (MC) calculations for charged particles (ions and electrons) confined by a 2D parabolic [6, 7] and by a hard wall potentials [8, 9] for small and large systems. Structures of polygonal patterns, similar to ones obtained in the effective harmonic oscillator confinement, have been observed in experimental measurements [10, 11]. Note, that in many cases, the polygonal pattern of equally charge particles is sufficiently regular.

The purpose of this contribution is to discuss a semi-analytical approach for analysis of ground state properties of charged particles in a disk as a function of particle number. We consider particles interacting by means of the Coulomb interaction at zero temperature in order to avoid the admixture of metastable states to the ground state. We will illuminate specific properties which distinguish the electronic configurations in the circular potential from the parabolic one.

2. Coulomb nteraction of rings

The Coulomb energy of n unit charges e forming a regular polygon [ring] has the following form [5]:

$$E_n(R) = \frac{n\,S_n\,e^2}{4\,R}\,, \qquad S_n = \sum_{k=1}^{n-1} \frac{1}{\sin\frac{\pi}{n}k}\,. \tag{1}$$

Evidently, one needs to know the interaction between rings. As it was shown in [12], the interaction between two rings with n and m charges is determined as:

$$E_{nm}(r_1, r_2, \psi) = \sum_{i=1}^{n}\sum_{j=1}^{m} \epsilon(r_1, r_2, \psi_{ij}^{nm} + \psi) = \mathrm{G} \times \sum_{k=1}^{\mathrm{L}} \epsilon(r_1, r_2, \psi_k + \psi)\,, \tag{2}$$

$$\epsilon(r_1, r_2, \theta) = (r_1^2 + {r_2}^2 - 2\,r_1\,r_2\,\cos\theta)^{-1/2}\,, \tag{3}$$

where $\psi_{ij}^{nm} = 2\,\pi(i/n - j/m)$, ψ is the relative angular offset between the two rings. Here, $\{\psi_k = \Delta \times k, k = 1, \ldots, L\}$; $L \equiv \mathrm{LCM}(n, m)$ and $G \equiv \mathrm{GCD}(n, m) = n \times m/L$ are the least common multiple and greatest common divisor of the of numbers (n, m), respectively. The energy is a periodic function with a $\Delta = 2\pi/L$ periodicity. In turn, this result shows that these kind of functions are invariant under angle transformations corresponding to the cyclic group of L elements.

Let us denote $r(R) = \min(\max)(r_1, r_2)$. Employing the expansion $\epsilon(1, x, \psi) = \Sigma_{l\geq 0} x^l\,P_l(\cos\psi)$, we obtain

$$E_{nm} = \langle E_{nm}\rangle + \Delta E_{mn}, \tag{4}$$

$$\Delta E_{mn} = R^{-1}\,(n\,m)\sum_{k=1}^{\infty} H_k(r/R)\,(r/R)^{k\times \mathrm{L}}\,\cos\left(k \times \mathrm{L}\,\psi\right) \tag{5}$$

Here, a zero order harmonic term is defined as

$$\langle E_{nm}\rangle \equiv \langle E_{nm}(r_1, r_2)\rangle = \frac{2\,n\,m\,K(4\,r_1\,r_2/(r_1 + r_2)^2)\,e^2}{\pi\,R} = \frac{2\,n\,m\,K((r/R)^2)\,e^2}{\pi R}\,, \tag{6}$$

and

$$H_k(x) = h_{k,\mathrm{L}}\,{}_2F_1(\tfrac{1}{2},\,\tfrac{1}{2} + k \times \mathrm{L},\,1 + k \times \mathrm{L};\,x^2), \tag{7}$$

$$h_{k,\mathrm{L}} = [2^{k\times \mathrm{L}}\,(k \times \mathrm{L})!]^{-1}\,2\,(2\,k\,\mathrm{L} - 1)!!\,. \tag{8}$$

Since $r/R < 1$, it is enough to consider only a leading term in the sum (5)

$$\Delta E_{mn} \approx \frac{nm}{R}\,H_1(r/R)\,(r/R)^L\,\cos(\mathrm{L}\,\psi), \qquad H_1(r/R) \approx h_{1,L} \tag{9}$$

3. Equilibrium configurations

The total energy is defined as

$$E_{\rm tot}(\mathbf{n},\mathbf{r},\psi)=\sum_{i=1}^{p}E_{n_i}+\sum_{i=2}^{p}\sum_{j=1}^{i-1}E_{n_in_j}(r_i,r_j,\psi_i-\psi_j)\,, \tag{10}$$

where a particle number $n=n(\mathbf{n})=\Sigma_{i=1}^{p}n_i$, p is a number of rings for a configuration $\mathbf{c}=(\mathbf{n},\mathbf{r},\psi)$. The numerical analysis [12] demonstrates that

$$E_{n_i,n_j}(r_i,r_j,\psi_i-\psi_j)\approx\langle E_{n,m}(r_i,r_j)\rangle, \tag{11}$$

holds for $n\leq 2000$ with a high accuracy. The equilibrium configuration of particles can be obtained by minimizing Eq.(10) with respect to $(p,\mathbf{n},\mathbf{r})$, i.e., finding the partition corresponding to the lowest total energy. For a given partition, the set of equations that determines the optimal radiuses $(r_i, i=2,\ldots,p)$ is

$$r_i^2\sum_{j=i+1}^{p}\frac{n_j\,{\rm E}((r_j/r_i)^2)}{{r_j}^2-r_i^2}+r_i\sum_{j=1}^{i-1}n_j\Big(\frac{r_j\,{\rm E}((r_i/r_j)^2)}{r_j^2-r_i^2}-\frac{{\rm K}((r_i/r_j)^2)}{r_j}\Big)=\frac{\pi}{8}S_{n_i}\,, \tag{12}$$

where ${\rm K}={\rm X}_{-1}$, ${\rm E}={\rm X}_1$ are complete elliptic integrals of first (second) kind:${\rm X}_p(x)=\int_0^{\pi/2}dt\,(1-x\,\sin^2 t)^{-p/2}$.

It is enough a few iterations of Eq.(12) to reach an optimal energy configuration (10) for a given partition. Making a grid of different partitions one can readily find the equilibrium configuration for a total number n.

4. Structure of magic configurations

The minimization of energy with respect to the ring's partition numbers $\mathbf{n}$ leads to the following "magic configurations":

11 :	11								
29 :	6	23							
55 :	5	13	37						
90 :	5	12	20	53					
135 :	5	12	19	29	70				
186 :	5	12	19	26	37	87			
246 :	5	12	18	25	34	46	106		
316 :	5	11	18	25	33	42	56	126	
394 :	5	11	18	25	32	40	50	66	147

(13)

These configurations are characterized with complete p shells. For example, for $n=394$ we obtain $p=9$ filled shells. The addition of one electron creates a *centered core configurations* with a number of electrons $6k, k=1,2,3\ldots$, starting from the one particle in the center

12 :	1	11							
30 :	1	6	23						
56 :	**1**	**6**	**12**	37					
92 :	**1**	**6**	**12**	20	53				
136 :	**1**	**6**	**12**	19	28	70			
187 :	**1**	**6**	**12**	**18**	26	37	87		
248 :	**1**	**6**	**12**	**18**	25	34	46	106	
317 :	**1**	**6**	**12**	**18**	25	32	42	55	126
395 :	**1**	**6**	**12**	**18**	**24**	32	40	50	65	147.

(14)

As a result, a new shell appears which is filling by electrons. The sequence of electrons in the filled shells of the *centered core configurations* is a characteristic property of the hexagonal lattice. It signals on the onset of the crystalliztion in the disk geometry for $n \geq 200$.

5. Asymptotic limit: $n \gg 1$

The density of the hexagonal lattice is defined as $\rho = c/a^2 e$, where $c = 2/\sqrt{3}$ and a is the distance between two nearest neighbor particles. At large n one can define this distance as $a = R/p$. As a result, one obtains

$$\rho = ne/\pi R^2 \Rightarrow p^2 \approx \frac{\sqrt{3}}{2\pi} \times n \tag{15}$$

To consider the density of the ring we employ the factorization of ϱ: $\varrho(r,\phi) = \rho(r) \times (2\pi)^{-1}$ which leads to a normalization of a radial integral: $Q = \int_0^R dr r\, \rho_R(r)$.

The distribution $\rho_R(r)$ can be obtained from the Ritz problem of the minimization of the Coulomb energy on a two–dimensional disk of radius R. To this aim we consider the functional $G_{[\rho]} = E_{[\rho]} g(V^0_{[\rho]})$ where

$$E_{[\rho]}(r) = \int_0^R dr\, A_{[\rho]}(r)\, \rho(r) = \int_0^R dr\, B_{[\rho]}(r)\, \rho(r), \tag{16}$$

$$A_{[\varrho]}(r) = c_0 \int_0^r dy\, y\, \mathrm{K}((y/r)^2)\, \varrho(y), \qquad B_{[\varrho]}(r) = c_0\, r \int_r^{\bar{R}} dy\, \mathrm{K}((r/y)^2)\, \varrho(y), \tag{17}$$

$$V^0_{[\rho]} = \int_0^R dr\, r\, \rho(r). \tag{18}$$

Hence the variational principle $\delta E_{[\rho]} = 0$ gives

$$0 = (A_{[\varrho]} + B_{[\varrho]})(r) + (E/g)\, g'(V^0)\, r\,, \tag{19}$$

where $c_0 = 2/\pi$. Since the integration of r.h.s. over r gives $2\,E + (E/g)\, g'(V^0)\, V^0$, the solution exists only if $g(x) = x^{-2}$. Denoting $X_m(z) = R^{-2}\, X_{[\varrho_m]}(z)\, (X = A, B)$, where $\varrho_m(r) = (r/R)^m = z^m$, we obtain

$$\begin{pmatrix} A_m(z) \\ B_m(z) \end{pmatrix} = \sum_{n=0}^{\infty} K_n \begin{pmatrix} \frac{z^{m+2}}{2+2\,n+m} \\ \frac{z\, h^m_n(z)}{1-2\,n+m} \end{pmatrix} = \begin{pmatrix} 0 \\ \frac{z\, \tilde{B}_m(z^2)}{m+1} \end{pmatrix} + \begin{pmatrix} \frac{z^{2+m}\, \tilde{A}_m(1)}{2+m} \\ \frac{-z^{m+2}\, \tilde{B}_m(1)}{1+m} \end{pmatrix}. \tag{20}$$

Here

$$K_n = \frac{((2\,n-1)!!)^2}{2^{2\,n}\, ((n)!)^2}, \qquad h^m_n(z) = z^{2\,n} - z^{1+m}, \tag{21}$$

$$\tilde{A}_m(z) = {}_3F_2(\tfrac{1}{2}, \tfrac{1}{2}, 1 + \tfrac{m}{2};\, 1, 2 + \tfrac{m}{2};\, z), \quad \tilde{B}_m(z) = {}_3F_2(\tfrac{1}{2}, \tfrac{1}{2}, -\tfrac{1+m}{2};\, 1, \tfrac{1-m}{2};\, z),$$

are considered for $m = 0, 2, \ldots$. Eq.(20) leads to the following condition

$$0 = (m+1)\, \tilde{A}_m - (m+2)\, \tilde{B}_m(1) \Longrightarrow A_m(z) + B_m(z) = (m+1)^{-1}\, z\, \tilde{B}_m(z^2). \tag{22}$$

The l.h.s. is a nontrivial identity fulfilled by generalized hypergeometric functions ${}_3\mathrm{F}_2$. Expanding $\varrho = \varrho(\mathbf{a})$ in series

$$\varrho(\mathbf{a}) = (Q/R^2) \times \sum_{n=0}^{\infty} a_n\, (r/R)^{2\,n} \tag{23}$$

and employing Eq.(22), we rewrite Eq.(19) in the form

$$z\left(\sum_{m=0}^{\infty} a_m\,(2\,m+1)^{-1}\,\tilde{B}_{2\,m}(z^2)-2\,(R/Q^2)\,E_{[\varrho]}\right)\,Q=0. \tag{24}$$

Evidently, $z\neq 0$, and, therefore, we obtain

$$E(\mathbf{a})=\frac{Q^2}{2\,R}\times\sum_{m=0}^{\infty}\frac{a_m}{2\,m+1}, \tag{25}$$

$$1=Q^{-1}\,Q_{[\varrho(\mathbf{a})]}=\sum_{m=0}^{\infty}\frac{a_m}{2\,m+2}=F_0(\mathbf{a}), \tag{26}$$

$$F_\alpha(\mathbf{a})=R^{-2\,\alpha}\,\langle r^{2\,\alpha}\rangle_\rho=\sum_{m=0}^{\infty}\frac{a_m}{2\,m+2\,\alpha+2}. \tag{27}$$

We require that the higher order terms in the sums in Eqs.(25) are zeros, and obtain:

$$F_{-(2\,\alpha+1)/2}(\mathbf{a})=0,\qquad \alpha=1,2,\ldots,\qquad E(\mathbf{a})=\frac{Q^2}{2\,R}\times F_{-1/2}(\mathbf{a})/F_0(\mathbf{a}), \tag{28}$$

As a result, we have

$$a_m=(-1)^m\binom{-1/2}{m}. \tag{29}$$

This result is consistent with the Taylor expansion of

$$\rho_R(r)=Q\,R^{-1}(R^2-r^2)^{-1/2}. \tag{30}$$

For finite n, the minimal energy E_n contains a smooth part. The numerical results are well fitted by series

$$E_{(\mathbf{a},\mathbf{b})}(n)\approx\frac{(ne)^2}{R}\left(\frac{\pi}{4}+\sum_{k=1}^{p}a_k/n^k+\sum_{k=1}^{q}b_k\,n^{-k}\,\ln n\right). \tag{31}$$

Here, the coefficient $a_0=\pi/4$ is found from Eq.(25) , takng into account that

$$\Sigma_{m=0}^{\infty}\,a_m/(2\,m+1)=\pi/2. \tag{32}$$

For finite (p,q), the "effective coefficients" $(\mathbf{a},\mathbf{b})$ could be fitted by a minimization:

$$\Sigma_n{\delta_n}^2\,,\qquad \delta_n=(E_n-E_{(\mathbf{a},\mathbf{b})}(n))\,R/(en)^2 \tag{33}$$

In the interval $n\in[20,400]$ a good estimation is obtained for $(p,q)=(4,3)$, which is

$$\binom{\mathbf{a}}{\mathbf{b}}=\begin{pmatrix}76.7756,1266.32,-617.616,-745.263\\ -16.9075,-552.892,-1502.45\end{pmatrix} \tag{34}$$

6. Summary

The zero–harmonic limit, applied for the study of equilibrium states of finite number of charged particles in a disk, essentially reduces the optimization problem for the ground state configuration. The proposed method reproduces with a remarkable accuracy the results obtained with the aid of numerical simulation (see details in [12]).

Acknowledgments
This work was supported in part by Bogoliubov-Infeld program of BLTP and RFBR grant 14-02-00723.

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