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A tendency to a formation of two-dimensional self-consistent structures in Coulomb systems

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Abstract. A class of periodic solutions of the two-dimensional Poisson–Boltzmann system was found. These Jacobi elliptic functions reveal a tendency to self-organisation, e.g. periodic spatial distribution, for self-consistent Coulomb ensembles.

The spatial distribution of the particles in a two-component Coulomb gas can be described by the solutions of the non-linear Poisson–Boltzmann (PB) equation (Debye and Huckel 1923, Lampert 1985)

$$\Delta\psi = \sinh\psi \tag{1}$$

with

$$\psi = e\varphi/k_{\rm B}T \qquad X = fx \qquad Y = fy \qquad Z = fz$$

where φ is the self-consistent electrostatic potential, $f = (8\pi n_0 e^2/\varepsilon k_{\rm B}T)^{1/2}$ is the reciprocal Debye length, n_0 is the homogeneous particle concentration, T is the absolute temperature and e is the electron charge. The spatial distribution of the positive and negative particle concentration, respectively n_+ and n_- in the thermal equilibrium can be determined by the Boltzmann law, using the solution ψ of the PB equation:

$$n_+ = n_0 \exp(-\psi) \tag{2}$$

$$n_- = n_0 \exp(\psi). \tag{3}$$

As has been shown (Martinov *et al* 1984, Georgiev *et al* 1980, 1986) the exponentially non-linear equation (1) in the plane symmetry case posseses an infinite number of periodic solutions with periods from 0 to ∞. As a result we obtain a periodic distribution of the particles of the system and the formation of a static plane wave of the space charge within it. It must be outlined that the existence of the periodic solutions is thus a direct consequence of the non-linearity of the PB equation. In the classical linear Debye–Huckel (1923) theory based on the linear variant of the PB equation, there are no periodic solutions and the tendency for periodic structure formation cannot be revealed. In this case we have only a monotonous decreasing solution.

In this paper the two-dimensional PB equation

$$\frac{\partial^2\psi}{\partial X^2} + \frac{\partial^2\psi}{\partial Y^2} = \sinh\psi \qquad \psi(X, Y) \tag{4}$$

will be studied and it will be shown that this equation possesses periodic solutions leading to self-consistent Coulomb structures with a corresponding symmetry.

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The substitution

$$\psi(X, Y) = 4\tanh^{-1}\left(\frac{\bar{u}(X)}{\bar{v}(Y)}\right) \qquad \begin{aligned}\bar{u}(X) &= Au(\alpha X)\\ \bar{v}(Y) &= v(\beta Y)\end{aligned} \tag{5}$$

as we shall see later makes it possible to separate the variables in (4). Here α and β are parameters. Assuming

$$\sinh\psi = \sinh(4\theta) = \frac{4\tanh(\theta)(1+\tanh^2(\theta))}{(1-\tanh^2(\theta))^2}$$

where $\theta = \tanh^{-1}(\bar{u}(X)/\bar{v}(Y))$, the result for the differential equation (4) is

$$\left(\alpha^2\frac{u''}{u} - \beta^2\frac{v''}{v}\right) + 2\frac{A\alpha^2(u')^2 + \beta^2(v')^2}{V^2 - A^2u^2} = \frac{v^2 + A^2u^2}{v^2 - A^2u^2}. \tag{6}$$

By appropriate differentiation of (6) by x and y, the following two equations may result:

$$\frac{\alpha^2}{A^2uu'}\left(\frac{u''}{u}\right)' = 4\left[\frac{v^2}{(v^2 - A^2u^2)^2} - \alpha^2\left(\frac{u''}{u}\right)\frac{(v^2 - A^2u^2)}{(v^2 - A^2u^2)^2} - \frac{A^2\alpha^2(u')^2 + \beta^2(v')^2}{(v^2 - A^2u^2)^2}\right) \tag{7a}$$

$$\frac{\beta^2}{vv'}\left(\frac{v''}{v}\right)' = 4\left(\frac{A^2u^2}{(v^2 - A^2u^2)^2} + \beta^2\left(\frac{v''}{v}\right)\frac{(v^2 - A^2u^2)}{(v^2 - A^2u^2)^2} - \frac{A^2\alpha^2(u')^2 + \beta^2(v')^2}{(v^2 - A^2u^2)^2}\right). \tag{7b}$$

Considering the summation of equations (7a) and (7b) and taking into account equation (6) produces the following non-linear equation:

$$\frac{\alpha^2}{A^2uu'}\left(\frac{u''}{u}\right)' + \frac{\beta^2}{vv'}\left(\frac{v''}{v}\right)' = 0. \tag{8}$$

The resulting equation (8) clearly defines the possibility of separating the variables in equation (4)

$$\frac{\alpha^2}{A^2uu'}\left(\frac{u''}{u}\right)' = -\frac{\beta^2}{vv'}\left(\frac{v''}{v}\right)' = -C = \text{constant}. \tag{9}$$

Therefore we reduce the non-linear partial differential equation (4) to two non-linear ordinary differential equations of third order

$$\frac{\alpha^2}{A^2uu'}\left(\frac{u''}{u}\right)' = -C \tag{10a}$$

$$\frac{\beta^2}{vv'}\left(\frac{v''}{v}\right)' = C. \tag{10b}$$

Integration of (10a) and (10b) leads to

$$(u')^2 = -\left(\frac{A^2C}{4\alpha^2}\right)u^4 + \left(\frac{\gamma_1}{\alpha^2}\right)u^2 + \left(\frac{\gamma_2}{\alpha^2}\right) \tag{11a}$$

$$(v')^2 = \left(\frac{C}{4\beta^2}\right)v^4 + \left(\frac{\delta_1}{\beta^2}\right)v^2 + \left(\frac{\delta_2}{\beta^2}\right) \tag{11b}$$

where γ_1, γ_2, δ_1, δ_2 are integration constants. Equations (11*a*) and (11*b*) are of the following type:

$$(u')^2 = a_1 u^4 + b_1 u^2 + c_1 \tag{12a}$$

$$(v')^2 = a_2 v^4 + b_2 v^2 + c_2 \tag{12b}$$

where the prime denotes differentiation by the corresponding variable.

Equations (12*a*) and (12*b*) generate the Jacobi elliptic functions and hence the solutions can be expressed in these functions. Satisfying equation (6) and taking into account (7*a*) and (7*b*), respectively (10*a*) and (10*b*), requires the following three conditions:

$$\begin{aligned} &\alpha^2 b_1 + \beta^2 b_2 = 1 \\ &\alpha^2 a_1 + A^2\beta^2 c_2 = 0 \\ &\beta^2 a_2 + A^2\alpha^2 c_1 = 0. \end{aligned} \tag{13}$$

The first condition in (13) we shall call the selection rule for the elliptic functions, the other two being commutation rules for the elliptic functions.

The coefficients a_i, b_i, c_i $(i = 1, 2)$ depend on the concrete elliptic function $u = u(\alpha X_1 k_1)$, $v = v(\beta Y, k_2)$ where k_1 and k_2 are the corresponding elliptic integral modules. The combination of elliptic functions $u(\alpha X_1, k_1)v(\beta Y, k_2)$ satisfying (4) can be determined by the dispersion relations (13). As can be seen from (13) these are couples of functions, for which the coefficients a_1 and c_2 must possess an opposite sign, respectively a_2 and c_1 for the real values of the parameters α, β, A.

The solution of equation (4) depends on the five constants A, α, β, k_1, k_2, among which the three relations (13) exist. Consequently it depends on two free parameters.

Table 1 below illustrates in detail the possible elliptic function combinations which satisfy equation (4). Combining table 1 and the conditions (13), the following seven possible types of the equation solutions are obtained, describing two-dimensional

Table 1. Relation between the modules of the 12 main Jacobi elliptic functions and the coefficients a, b, c in their generating equations.

Elliptic function	a	b	c
cn x	$-k^2$	$2k^2-1$	$1-k^2$
sn x	k^2	$-1-k^2$	1
dn x	-1	$2-k^2$	k^2-1
sn x/cn x	$1-k^2$	$2-k^2$	1
cn x/sn x	1	$2-k^2$	$1-k^2$
sn x/dn x	$-k^2(1-k^2)$	$2k^2-1$	1
dn x/sn x	1	$2k^2-1$	$-k^2(1-k^2)$
cn x/dn x	k^2	$-1-k^2$	1
dn x/cn x	1	$-1-k^2$	k^2
$(\mathrm{sn}\,x)^{-1}$	1	$-1-k^2$	k^2
$(\mathrm{cn}\,x)^{-1}$	$1-k^2$	$2k^2-1$	$-k^2$
$(\mathrm{dn}\,x)^{-1}$	k^2-1	$2-k^2$	-1

periodic structures with periods T_X and T_Y respectively.

$$\psi = 4\tanh^{-1}[A\,\mathrm{cn}(\alpha X, k_1)\,\mathrm{cn}(\beta Y, k_2)]$$

$$k_1^2 = \frac{A^2[\alpha^2(A^2-1)-1]}{\alpha^2(A^2-1)^2} \qquad k_2^2 = \frac{A^2[\beta^2(A^2-1)-1]}{\beta^2(A^2-1)^2} \tag{14}$$

$$\alpha^2+\beta^2 = \frac{A^2+1}{A^2-1} \qquad T_X = \frac{4K(k_1)}{\alpha} \qquad T_Y = \frac{4K(k_2)}{\beta}$$

$$\psi = 4\tanh^{-1}\left(Ak_1'k_2'\frac{\mathrm{sn}(\alpha X/k_1', k_1)}{\mathrm{dn}(\alpha X/k_1', k_1)}\frac{\mathrm{sn}(\beta Y/k_2', k_2)}{\mathrm{dn}(\beta Y/k_2', k_2)}\right)$$

$$k_1^2 = \frac{A^2\alpha^2(A^2-1)}{\alpha^2(A^2-1)^2-1} \qquad k_2^2 = \frac{A^2\beta^2(A^2-1)}{\beta^2(A^2-1)-1} \tag{15}$$

$$\alpha^2+\beta^2 = \frac{1}{A^2-1} \qquad T_X = \frac{4K(k_1)k_1'}{\alpha} \qquad T_Y = \frac{4K(k_2)k_2'}{\beta}$$

$$\psi = 4\tanh^{-1}\left(A\,\mathrm{cn}(\alpha X, k_1)\frac{\mathrm{sn}(\beta Y/k_2', k_2)}{\mathrm{dn}(\beta Y/k_2', k_2)}\right)$$

$$k_1^2 = \frac{A^2[\alpha^2(A^2-1)-1]}{\alpha^2(A^2-1)^2} \qquad k_2^2 = \frac{A^2[1-\beta^2(A^2-1)]}{A^2-\beta^2(A^2-1)^2} \tag{16}$$

$$\alpha^2-\beta^2(A^2-1) = \frac{1}{A^2-1} \qquad T_X = \frac{4K(k_1)}{\alpha} \qquad T_Y = \frac{4K(k_2)k_2'}{\beta}$$

$$\psi = 4\tanh^{-1}\{A\,\mathrm{dn}(\alpha X, k_1)\,\mathrm{sn}(\beta Y, k_2)\}$$

$$k_1^2 = 1-\frac{\alpha^2/A^2(A^2-1)-1}{\alpha^2(A^2-1)} \qquad k_2^2 = \frac{A^2[\beta^2(A^2-1)-1]}{\beta^2(A^2-1)} \tag{17}$$

$$\alpha = A\beta \qquad T_X = \frac{2K(k_1)}{\alpha} \qquad T_X = \frac{4K(k_2)}{\beta}$$

$$\psi = 4\tanh^{-1}\left(A\,\mathrm{dn}(\alpha X, k_1)\frac{1}{\mathrm{sn}(\beta Y, k_2)}\right)$$

$$k_1^2 = \frac{\alpha^2(A^2-1)^2-A^2}{\alpha^2A^2(A^2-1)} \qquad k_2^2 = \frac{\beta^2(A^2-1)+A^2}{A^2\beta^2(A^2-1)} \tag{18}$$

$$\alpha^2-\beta^2 = \frac{A^2}{A^2-1} \qquad T_X = \frac{2K(k_1)}{\alpha} \qquad T_Y = \frac{4K(k_2)}{\beta}$$

$$\psi = 4\tanh^{-1}\left(A\,\mathrm{dn}(\alpha X, k_1)\frac{\mathrm{sn}(\beta Y, k_2)}{\mathrm{cn}(\beta Y, k_2)}\right)$$

$$k_1^2 = \frac{\alpha^2/A^2(1+A^2)-1}{\alpha^2(1+A^2)}+1 \qquad k_2^2 = 1-\frac{A^2[1-\beta^2(1+A^2)]}{\beta^2(1+A^2)} \tag{19}$$

$$\alpha = A\beta \qquad T_X = \frac{2K(k_1)}{\alpha} \qquad T_Y = \frac{4K(k_2)}{\beta}$$

$$\psi = 4\tanh^{-1}\left(A\,\mathrm{dn}(\alpha X, k_1)\frac{\mathrm{cn}(\beta Y, k_2)}{\mathrm{sn}(\beta Y, k_2)}\right)$$

$$k_1^2 = 1-\frac{1-\alpha^2/A^2(A^2+1)}{\alpha^2(A^2+1)} \qquad k_2^2 = 1-\frac{1-\beta^2/A^2(A^2+1)}{\beta^2(A^2+1)} \tag{20}$$

$$\alpha^2+\beta^2=\frac{A^2}{A^2+1} \qquad T_X=\frac{2K(k_1)}{\alpha} \qquad T_Y=\frac{4K(k_2)}{\beta}.$$

These seven types of solutions do not cover the wide variety of possible solutions of the two-dimensional PB equation based on elliptic functions. It can be shown that considerably more complicated algebraic combinations of elliptic functions satisfy the equation of the following type:

$$\left(\frac{\mathrm{d}u}{\mathrm{d}x}\right)^2=au^4+bu^2+c. \tag{21}$$

Such functions are the following:

$$\begin{aligned}
&\psi_1(X)=\frac{1-k_1\,\mathrm{sn}^2(\alpha X,k_1)}{1+k_1\,\mathrm{sn}^2(\alpha X,k_1)}\\
&a=-(1+k_1)^2 \qquad b=2(1+k_1)^2-4k_1 \qquad c=4k_1-(1+k_1)^2\\
&\psi_2(Y)=(1+k_2')\frac{\mathrm{sn}(\beta Y,k_2)\,\mathrm{cn}(\beta Y,k_2)}{\mathrm{dn}(\beta Y,k_2)}\\
&a=\frac{k_2^4}{(1+k_2')^2} \qquad b=-2(2-k_2^2) \qquad c=(1+k_2')^2.
\end{aligned} \tag{22}$$

This allows us to build a solution of equation (4), differing from the seven solutions given above, or

$$\psi=4\tanh^{-1}[A\psi_1(X)\psi_2(Y)]. \tag{23}$$

Consequently the variety of the solutions of equation (4) is very wide. The solutions (14)-(20) presented above possess some common properties, which are now presented.

A general property for all possible solutions is the fact that, when fixing the period in one direction (for example T_X) or assigning some values to k_1 and α, the self-consistent two-dimensional structures require a determined period in the other direction. Therefore the solutions cannot possess an arbitrary period in the other direction. In a particular case, for example T_2, the periods can be infinite and the corresponding solution is expressed in elementary functions (it concerns the solution (14))

$$\psi=4\tanh^{-1}\left(A\cos(\alpha X)\frac{1}{\cosh(\beta Y)}\right) \qquad \alpha^2=\frac{1}{A^2-1} \qquad \beta^2=\frac{A}{A^2-1} \tag{24}$$

where $T_X=2\pi/\alpha$, $T_Y=\infty$. This one-periodic solution of the PB equation can be obtained formally from (14) setting $k_1=0$ and $k_2=1$. In accordance with the above it must be mentioned that equation (4) does not possess a solution of type (5) non-periodic in both directions. For the solution (14), the condition for α, β, A to be real requires $\infty > A \geqslant 1$; hence the following relation between k_1 and k_2 may be obtained:

$$2>k_1^2+k_2^2\geqslant 1. \tag{25}$$

This inequality explains the above-mentioned properties of two-dimensional self-consistent solutions. All the solutions of equation (4) possess singularities for some values of the coordinates x and y. The points in the xy plane for which the solution possesses a singularity can be determined by the following condition: the argument of the $\tanh^{-1}$ function in (5) must be equal to ± 1. The form of a single line in the xy plane can be determined from this condition. The equation of this line in the first quadrant for the solution (14) is as follows:

$$A\,\mathrm{cn}(\alpha X,k_1)\,\mathrm{cn}(\beta Y,k_2)=1. \tag{26}$$

Of course the form of the line depends on the two free parameters of the solution. In the particular case $k_1=0$, $k_2=1$ (see solution (24)) the singular line is presented in figure 1 for different values of parameter A. For each solution this line is closed and it outlines an area, the size of which varies from zero to infinity.

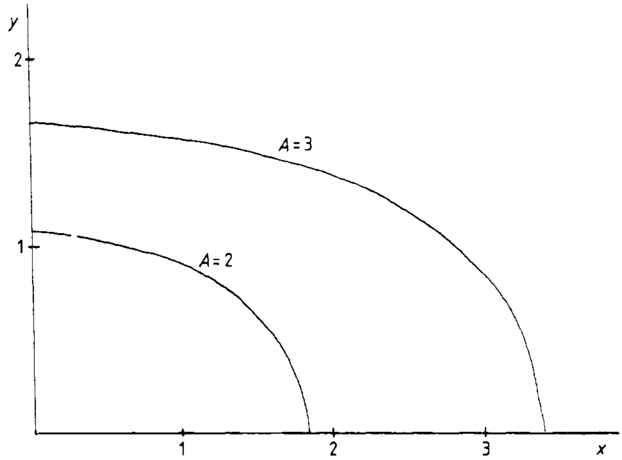

Figure 1. Form of the singularity line in the $x0y$ plane for solution (24) of the PB equation.

The solutions (14)-(20) presented above can be classified according to the type of space structure they describe. These two types of structure are illustrated in figures 2(a) and 2(b). Solutions (14), (15) and (16) may be referred to as of the first type, while solutions (17), (18), (19) and (20) are of the second type. Structure means a periodic self-consistent spatial distribution (see formulae (2) and (3)) of the Coulomb gas particle concentration.

Taking into account that the non-linear equation (4) is a scaling non-invariant, the conclusion may be that the transition from one type of solution to another can be performed by a scaling transformation. An analysis was performed to explain the scaling transformation properties of the solutions (14)-(20). As an example we shall perform the transition from solution (14) to solution (17), which can be accomplished by the scaling transformation

$$\begin{aligned} \mathrm{cn}(\alpha x, k_1) &\to \mathrm{dn}\left(\alpha k_1 x, \frac{1}{k_1}\right) \\ \mathrm{cn}(\beta y, k_2) &\to \mathrm{sn}\left(\beta k_2' y, \frac{ik_2}{k_2'}\right). \end{aligned} \tag{27}$$

As can be seen this transformation reforms the dispersion relations for the solution (14) into the relations for the solution (17). An interesting property of the two-dimensional solutions obtained is their relation to the Laplace equation two-dimensional periodic solutions. This connection can also be noticed in the spherical symmetry (Martinov *et al* 1985) solution of the linear Debye-Huckel equation for the self-consistent field

$$\varphi = (e/r)\,\mathrm{e}^{-fr}. \tag{28}$$

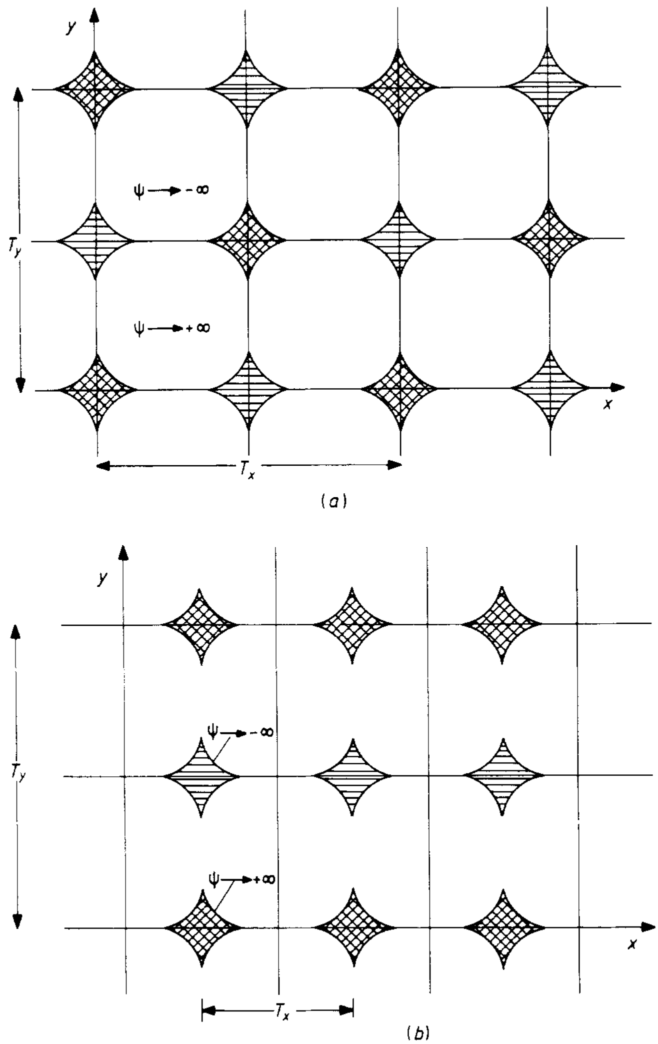

Figure 2. Two possible types of space structures, (*a*) type I, (b) type II, described by the solutions (14)-(20) of the PB equation. The hatched areas are framed by a line on which the potential ψ is $\pm\infty$.

The solution (28) is tending asymptotically to the solution

$$\varphi = e/r \tag{29}$$

of the radial symmetry Laplace equation, where fr is tending to 0. If we take for example the solution (1) and set $A=1$, $\alpha=\beta$, the corresponding dispersion relations reduce to a single relation

$$k_1^2 + k_2^2 = 1 \qquad k_2^2 = 1 - k_1^2 = k_1'^2 \tag{30}$$

and the function obtained

$$\psi_{\mathrm{L}} = 4 \tanh^{-1}[\mathrm{cn}(\alpha x, k_1)\,\mathrm{cn}(\alpha y, k_2)] \tag{31}$$

is a solution of the two-dimensional Laplace equation

$$\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}=0. \tag{32}$$

The analysis performed for solutions (14)-(20) shows that only some of them can be reduced to the two-dimensional periodic solutions of the Laplace equations.

The physical meaning of the solution (31) is given in Morse *et al* (1953). This solution describes a structure of positive and negative homogeneously charged infinite treads periodically distributed in the $x0y$ plane and oriented parallel to the $0z$ axis. The structure corresponding to solution (31) is given in figure 3.

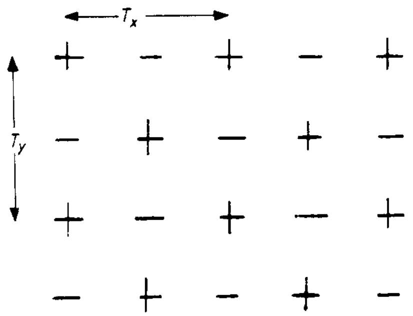

Figure 3. Spatial distribution of the charged treads leading to solution (31) of the Laplace equation $T_X=4k(k)/\alpha$, $T_Y=4k(k')/\alpha$.

As can be seen this figure is similar to figure 2(a). The singularities of the solution are localised on the treads in the case of the Laplace equation. For solution (14) of the PB equation the singularities arise over the cylindrical surfaces parallel to the $0z$ axis. The form of the base of these cylindrical surfaces can be determined by equation (25). These cylindrical surfaces are distributed periodically in space (figures 2(a) and 2(b)). If the parameter $A\to 1$ these cylinders reduct to charged lines.

The presence of the singularities in the solutions of the Laplace equation as in the solutions of the non-linear PB equation is a consequence of the existence of charged treads and, respectively, surface charge density. These particular properties of the solutions of the Laplace equation are introduced 'artificially' by a periodic distribution of x charged treads. In the case of the PB equation they reveal an inherent property of the self-consistent system. This tendency for structure in the two-dimensional Coulomb gas results directly from the non-linearity of the PB equation and must be considered as a characteristic self-organisation of this system.

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