PAPER

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Monte Carlo simulations of two-component Coulomb gases applied in surface electrodes

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Abstract

In this work, we study the gapped surface electrode (SE), a planar system composed of two-conductor flat regions at different potentials with a gap $\mathcal{G}$ between both sheets. The computation of the electric field and the surface charge density requires solving Laplace's equation subjected to Dirichlet conditions (on the electrodes) and Neumann boundary conditions over the gap. In this document, the gapless surface electrode is modeled as a two-dimensional classical Coulomb gas having punctual charges $+q$ and $-q$ on the inner and outer electrodes, respectively, interacting with an inverse power law $1/r$-potential. The coupling parameter Γ between particles inversely depends on temperature and is proportional to q^2. Precisely, the density charge arises from the equilibrium states via Monte Carlo (MC) simulations. We focus on the coupling and the gap geometry effect. Mainly on the distribution of particles in the circular and the harmonically-deformed gapped SE. MC simulations differ from electrostatics in the strong coupling regime. The electrostatic approximation and the MC simulations agree in the weak coupling regime where the system behaves as two interacting ionic fluids. That means that temperature is crucial in finite-size versions of the gapped SE where the density charge cannot be assumed fully continuous as the coupling among particles increases. Numerical comparisons are addressed against analytical descriptions based on an electric vector potential approach, finding good agreement.

Keywords: MC simulations, two-component plasma, surface electrode, Biot–Savart law, long-range interaction potential

(Some figures may appear in colour only in the online journal)

1. Introduction

The gapped surface electrode (SE) is a device composed of two infinite conductor sheets laying on the xy-plane. One of these sheets is located in the $\mathcal{A}_{\text{in}}$ region and has a constant potential V_0. The second one is a grounded region $\mathcal{A}_{\text{out}}$ having null potential, which is separated from the potential region by a gap $\mathcal{G}$ (see figure 1-left). The main problem here is to determine the electric field $\boldsymbol{E}$ in the $\mathbb{R}^3$-space and the density charge distribution $\sigma(x, y)$ on the sheets. In general, these quantities depend strongly on the gap region:

$$\mathcal{G} = \{(r, \phi, 0) : \quad \mathscr{R}(\phi) - \nu/2 < r < \mathscr{R}(\phi) + \nu/2 \quad \forall \quad \phi \in [0, 2\pi)\},$$

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with $(\mathscr{R}(\phi),\phi)$ and $(\mathscr{R}(\phi)\pm\nu/2,\phi)$ the parametric representations of contours ∂A and $\partial A_{\pm}$,[5] respectively.

The mathematical problem requires to solve a Laplace's equation for the scalar electric potential $\Phi(\boldsymbol{r})$ given by

$$\nabla^2\Phi(\boldsymbol{r})=0,\quad \boldsymbol{r}\in\mathfrak{D}=\left\{\boldsymbol{r}\in\mathbb{R}^3:z>0\right\},\tag{1}$$

subjected to the following Dirichlet and Neumann boundary conditions:

$$\Phi(\boldsymbol{r})=V_0\quad \textbf{if } \boldsymbol{r}\in\mathcal{A}_{\text{in}}\subset\left\{\boldsymbol{r}\in\mathbb{R}^2:z=0\right\},\tag{2}$$

$$\Phi(\boldsymbol{r})=0\quad \textbf{if } \boldsymbol{r}\in\left\{\boldsymbol{r}\in\mathbb{R}^2:z=0\right\}\setminus\mathcal{A}_{\text{in}}\cup\mathcal{G},\tag{3}$$

$$\frac{\partial\Phi(\boldsymbol{r})}{\partial z}=0\quad \textbf{if } \boldsymbol{r}\in\mathcal{G}.\tag{4}$$

In general, this problem does not have an analytic solution. One alternative is to obtain $\boldsymbol{E}$ and σ through the electric vector potential $\boldsymbol{\Theta}$. That alternative relies on the divergenceless condition of the electric field in the free charge region and the fact that $\boldsymbol{E}=\nabla\times\boldsymbol{\Theta}$. The approach adopts an analogy of the SE with magnetostatics and it is particularly viable when the solution of the gapless problem is known exactly[6]. Even with numerical methods e.g. finite element methods (FEMs) or finite difference methods the approximation to (1)–(4) is not trivial, mostly because of the mixture of Dirichlet and Neumann boundary conditions and the discontinuity of $\partial_z\Phi$ at the electrodes boundaries $\partial A_{\pm}$. This system is often used as a model to study of surface-electrode (SE) Radio Frequency ion traps. Those devices are a promising candidates to build ion-trap networks suitable for large-scale quantum processing [1–8]. The electrostatic SE is an ingredient of SE-ion traps. Typically, the surface-electrode trap includes control electrodes with static potentials alliterating them with RF electrodes. The electrostatic calculations are useful in the computations of such trapping potentials on real traps [9].

There are also analytical works describing SE in diverse geometries [10–12] which allow to approximate their charge distributions and electric field.

A possible physical description of this device is to define it as a Coulomb system. In particular, considering that electrons are particles that can move within the SE regions[7]. More specifically, by modeling the gapped SE as an ionic fluid with no mixing between charges. Hence, the SE can be thought as a system composed by $N/2$ positive point like charges on the inner electrode $\mathcal{A}_{\text{in}}$ and $N/2$ particles with opposite charge on the outer electrode $\mathcal{A}_{\text{out}}$. The system is globally neutral by definition[8] and particles can move freely in the electrode regions (see figure 1-right). The system can eventually converge to the electrostatic setting. That happens since a collective motion in a preferred direction may not occur[9]: macroscopically, the electric current on the electrodes is negligible $\boldsymbol{J}=0$. Moreover, electric charges in electrostatics are considered to be at rest and their thermodynamics does not play any role[10]. There are multiple models that can be chosen to represent this problem. One could be that of a fixed charge background and distributed moving positive charges on the electrodes. That would be like having two one-component plasmas, giving also a diversity of research possibilities. Since the net charge is the main objective, we use positives on one side of the electrode and negatives on the other. Instead of letting charges of both signs on the conductor sheets of the electrode, the one-type of particles leads to an accurate representation of the system.

In this document, we are interested in the effect of temperature on the SE by modeling it as a Coulomb system. Two-dimensional systems of interacting charge particles as fluids are commonly referred in the literature as two-dimensional plasmas (2dTCP), and one-component plasma 2dOCP if there is only a type of charge. For them, the coupling among particles plays a fundamental role on their collective behaviour. In fact, the thermodynamics of these systems is often described in terms of a coupling parameter Γ depending on the charge and the inverse of temperature. The current study attempts to model the gapped SE as a 2dTCP with no mixing, or conversely two interacting 2dOCP placed in two electrodes. The 2dOCP has been widely studied [13–19] because it is a simple system that mimic phase transitions [20–22] of real systems as dusty plasmas [23]. One of the peculiarities of these systems is that they form quasi-two-dimensional solids in the strong coupling regime ($\Gamma\to\infty$). In the case of the 2dOCP, a regular crystallization is found in a hexagonal crystal lattice, called the Wigner crystal. These plasma crystals have been experimentally achieved during the nineties [24, 25] by confining particles of several micrometers on horizontal layers.

The Monte Carlo (MC) technique in the canonical ensemble is adopted in this work. This description sufficiently represents the physics of the 2dTCP system in the gapless surface electrode (GSE). By scaling the solution, one can avoid the grand canonical ensemble in the MC simulations. This behavior is validated by means of analytical techniques: thermal averages can be directly compared to the surface charge density from the electrostatic analysis of the gapped SE. Moreover, the MC method allows simulating several coupling regimes of the system. On the contrary, the FEM solves the problem by modeling the gapped SE as an electrostatic problem. That approximation does not represent physics for the strong coupling regime. There are other methods such as molecular system dynamics [26, 27], electrohydrodynamics, evolutionary algorithms for the ground state [28], path integral algorithms [29], and

[5] We shall use the notation $\partial A_{-}=\partial A_{\text{in}}$, $\partial A_{+}=\partial A_{\text{out}}$ to denote the boundaries of the inner and outer electrodes, and ∂A for the mid path of the gap.

[6] The gapless problem solution occurs in the $\nu\to 0$ limit.

[7] Electrons (as electric charge carriers) are not fixed in stationary positions on a real conductor.

[8] No background density charge occurs on the flat sheets.

[9] It is known that a collective motion of electrons can generate an effective electric density current.

[10] In fact, electrostatics is an approximated model of conductors with no electric currents.

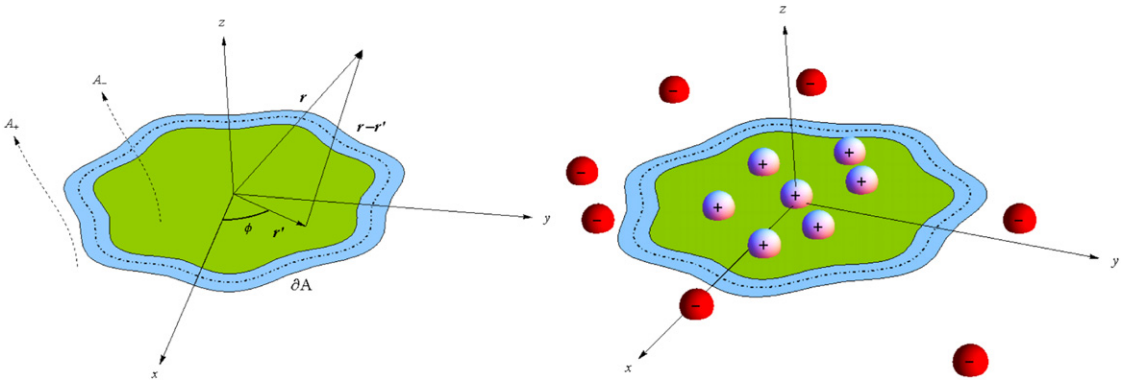

Figure 1. The electrostatic system. (Left) The gapped SE is composed of two flat sheets at different electric potentials separated by a gap in between. (Right) The SE is modeled as moving point-like particles of opposite charges with no mixing due to the gap.

differential equation approximation techniques to solve this type of 2dTCP system as well as other Coulomb systems.

In the solution techniques of Coulomb systems, it is necessary to consider the effect of the system boundaries. Especially when dealing with numerical solutions in finite systems such as the MC method. Crystalline structures occur in the ground state configuration for most one-component systems. Precisely, the boundary conditions of the system, or curved internal geometries, generally include defects in the crystalline structure. That causes the system to end up in non-crystalline configurations in the strong coupling regime. The gap in the GSE avoids the mixing between charges but also restricts the system to a non-crystalline structure. Physical boundaries are often avoided in Coulomb systems to prevent destroying the crystal. Specifically, MC simulations must carefully perform the inclusion of boundaries to represent the crystallization network of the particles. Periodic boundary conditions with adaptive domains on the crystal are one preferred technique.

This article is organized as follows. In section 2 we present an approach to solve the electrostatics of the system based on the electric vector potential formulation. Section 3 describes the numerical approximation using the MC method for SE with generic boundaries. We also present in that section simplifications on the thermodynamic averages computation due to the azimuthal symmetry of the circular SE. In section 4 the results numerical simulations of for the circular SE and harmonically deformed circular SE are presented. Those numerical results are contrasted with the electrostatic solution via the electric vector potential approach. Finally, in section 5 conclusions are given.

2. The electric vector potential formulation

The introduction of the electric vector potential $\boldsymbol{\Theta}$ is advantageous in the SE problem[11]. This is explained since it may considerably simplify the mathematical problem[12].

Using the Helmholtz decomposition theorem, the electric vector potential of the gapped SE can be obtained from [30] [13]

$$\boldsymbol{\Theta}(\boldsymbol{r}) = \frac{V_0}{2\pi}\int_{\mathscr{G}} \frac{\mathrm{d}^2\boldsymbol{r}'}{|\boldsymbol{r}-\boldsymbol{r}'|}\boldsymbol{\mathcal{W}}_\nu(\boldsymbol{r}'), \tag{5}$$

where the integration is defined on the gap region $\mathscr{G}$ and $\boldsymbol{\mathcal{W}}_\nu(u,\phi)$ is a weight vector whose components in the polar coordinates (u,ϕ) are

$$(\boldsymbol{\mathcal{W}}_\nu)_u = \frac{1}{V_0}\frac{1}{u}\frac{\partial\Phi_{\mathscr{G}}}{\partial\phi}(u,\phi), \quad \text{and} \quad (\boldsymbol{\mathcal{W}}_\nu)_\phi = -\frac{1}{V_0}\frac{\partial\Phi_{\mathscr{G}}}{\partial u}(u,\phi) \tag{6}$$

with $\Phi_{\mathscr{G}}$ the scalar electric potential in the gap. This two-dimensional weight vector is defined only on the gap region and it satisfies the $\nabla\cdot\boldsymbol{\mathcal{W}}_\nu(\boldsymbol{r}) = 0$ condition. The electric field can be obtained straightforwardly by applying the curl of equation (5). The result for $z > 0$ is

$$\boldsymbol{E}(\boldsymbol{r}) = \nabla\times\boldsymbol{\Theta} = \frac{V_0}{2\pi}\int_{\mathscr{G}}\frac{\boldsymbol{\mathcal{W}}_\nu(\boldsymbol{r}')\mathrm{d}^2\boldsymbol{r}'\times(\boldsymbol{r}-\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|^3}. \tag{7}$$

Equation (7) is mathematically analogue to the Biot–Savart law of magnetostatics. In fact, the gapped SE is the electrostatic analogue of a ribbon (on the gap region) carrying a steady density current $\mathscr{K}$ (see table 1). In general, the weight vector $\boldsymbol{\mathcal{W}}_\nu(\boldsymbol{r}')$ is unknown but it can be found by approximating the scalar potential in the gap Φ_{G} as

$$\Phi_{\mathrm{G}}(u,\phi) = \Phi_{\mathrm{SL}}(u,\phi) + \alpha(\phi)\xi_\nu(u,\phi), \tag{8}$$

where α is a parameter (see equation (10)), $\Phi_{\mathrm{SL}}(u)$ is the scalar potential of an infinite-straight and thick-gapped SE given by

[11] The electric field due to an electrostatic configuration is divergencesless $\nabla\cdot\boldsymbol{E} = 0$ and can be obtained from the identity $\boldsymbol{E} = \nabla\times\boldsymbol{\Theta}$.

[12] It is often preferred to use the scalar vector potential $\Phi(\boldsymbol{r})$ instead of the electric vector potential because it is more practical to deal with a scalar quantity. Not in the present case.

[13] This potential satisfies both the Coulomb gauge $\nabla\cdot\boldsymbol{\Theta}(\boldsymbol{r}) = 0$ in $\mathcal{D}$ and the $\boldsymbol{\Theta}(\boldsymbol{r})\cdot\hat{n} = 0$ gauge boundary condition on $\partial\mathcal{D}$, where $\mathcal{D} = \{\boldsymbol{r}\in\mathbb{R}^3 : z > 0\}$ and $\hat{n}(\boldsymbol{r})$ is the normal outward vector of $\partial\mathcal{D}$.

$$\Phi_{\rm SL}(u,\phi) = V_0\Pi_\nu(u,\phi)\left[\frac{1}{2} - \frac{1}{\pi}\arcsin\left(\frac{2(u-\mathcal{R}(\phi))}{\nu}\right)\right], \quad \text{and} \quad \xi_\nu(u,\phi) = V_0\Pi_\nu(u,\phi)\sqrt{1-\left[\frac{2}{\nu}(u-\mathcal{R}(\phi))\right]^2}$$

is a gap polarization potential. The $\Pi_\nu(u,\phi)$ function equals 1 on the gap region and 0 on the electrodes. The weight vector can be computed from equation (6) as follows

$$\boldsymbol{\mathcal{W}}_\nu(\boldsymbol{r}) = \frac{(\nu + 2\pi\alpha(u-\mathcal{R}(\phi)))}{\pi\nu^2 u\sqrt{1-\frac{4(u-\mathcal{R}(\phi))^2}{\nu^2}}}2(\dot{\mathcal{R}}(\phi)\hat{u} + u\hat{\phi}). \tag{9}$$

Equation (9) can be used to approximate the weight vector in the gap. To do so, it is necessary to calculate the α parameter with the zero density charge condition $\sigma = 0$ in the mid trajectory in the gap $\mathcal{R}(\phi)$. In polar coordinates, that refers to

$$\alpha(\phi) = -\frac{\frac{\pi}{\epsilon_0}\sigma^{\mathbf{GSE}}(\mathcal{R}\cos(\phi), \mathcal{R}\sin\phi; \mathcal{R}_-(\phi)) + J[\Phi_{\rm SL}](\mathcal{R}, \pi/2, \phi)}{J[\xi_\nu](\mathcal{R}, \pi/2, \phi)}, \tag{10}$$

where $\sigma^{\mathbf{GSE}}(x, y, \mathcal{R}_-(\phi))$ is the surface charge density in the gapless limit $\nu \to 0$ on the path $\partial\mathcal{A}_{\rm in}$, $\mathcal{R}_\pm(\phi) = \mathcal{R}(\phi) \pm \nu/2$ are the closed paths in polar coordinates that defines the electrodes borders $\partial A_\pm$, and

$$J[f](r,\theta,\phi) = \int_0^{2\pi} \mathrm{d}\phi' \int_{\mathcal{R}_-(\phi')}^{\mathcal{R}_+(\phi')} \frac{r^2(1-3\cos^2\theta) + u'^2 - 2ru'\cos(\phi-\phi')\sin\theta}{[r^2+u'^2-2ru'\cos(\phi-\phi')\sin\theta]^{5/2}} u'\,\mathrm{d}u'\,f(u').$$

2.1. The gapped circular SE

The gapped circular SE is defined by $\mathcal{R}(\phi) = R$ where the gap is an annular region of constant thickness $\nu = \Delta R$. Since the system is axially symmetric and the density charge is assumed as a continuous distribution, then $\sigma(x,y)$, $\boldsymbol{\Theta}(\boldsymbol{r})$, $\boldsymbol{E}(\boldsymbol{r})$, and $\Phi(\boldsymbol{r})$ do not depend on the ϕ-coordinate. One of the advantages of the circular SE is that the electrostatic field is known exactly in the gapless limit $\nu \to 0$, namely the GSE approximation. The electric vector potential of the GSE is given by [30]

$$\boldsymbol{\Theta}^{\mathbf{GSE}}(r,\theta) = \frac{V_0}{2\pi}\frac{4R}{\sqrt{R^2+r^2+2Rr\sin\theta}} \times \left[\frac{(2-\gamma^2)K(\gamma^2) - 2\tilde{E}(\gamma^2)}{\gamma^2}\right]\hat{\phi}, \tag{11}$$

where $\gamma^2(r,\theta) := 4Rr\sin\theta/(R^2+r^2+2Rr\sin\theta)$, and K and $\tilde{E}$ are the complete elliptic integrals of first and second kind, respectively. The electric field is obtained straightforwardly from the curl of equation (11), and the surface density charge is found by evaluating E_z in the limit $z \to 0$. The surface charge density of the circular GSE of radius R is

$$\begin{aligned}\sigma^{\mathbf{GSE}}(u;R) &= \frac{2\epsilon_0}{u}\lim_{\theta\to\frac{\pi}{2}}\frac{\partial}{\partial r}\left[r\Theta_\phi^{\mathbf{GSE}}(r,\theta)\right] \\ &= \frac{2\epsilon_0 V_0}{\pi}\left[\frac{1}{R-u}\tilde{E}\left(\frac{4Ru}{(R+u)^2}\right) + \frac{1}{R+u}K\left(\frac{4Ru}{(R+u)^2}\right)\right],\end{aligned} \tag{12}$$

with $u = \sqrt{x^2+y^2}$. The exact gapless solution given by equation (12) can be used to compute the density charge distribution of the gapped SE as follows,

$$\begin{aligned}\sigma(\boldsymbol{r}) &= \int_{R_-}^{R_+} (\mathscr{W}_\nu)_\phi(u'')\sigma^{\mathbf{GSE}}(\boldsymbol{r};u'')\mathrm{d}u'' \\ &= \left\langle (\mathscr{W}_\nu)_\phi(u''), \sigma^{\mathbf{GSE}}(\boldsymbol{r};u'')\right\rangle_{\mathcal{G}},\end{aligned} \tag{13}$$

which corresponds to a weight average of the gapless exact solution on $\mathcal{G}$, where $R_\pm := R \pm \nu/2$. Due to the azimuthal symmetry of the circular SE, the weight vector is given by equation (9), for which $(\mathscr{W}_\nu)_u = 0$.

For a discrete configuration $\mathscr{C}$ on the circular SE, the $\boldsymbol{\Theta}_{\mathscr{C}}(\boldsymbol{r})$ and $\boldsymbol{E}_{\mathscr{C}}(\boldsymbol{r})$ quantities are no longer independent of ϕ-coordinate. However, it is expected that the thermodynamic average of the charge density, as well as the fields, recover the axial symmetry. Therefore, we may still use this feature of the system in the electrostatic approximation and focus on the angular average of the discrete configurations.

2.2. Angular-averaged electric scalar potential

The potential at point $\boldsymbol{r} = (r,\theta,\phi)$ (in spherical coordinates) due to a $\mathscr{C}$ configuration with particles located at $\{\boldsymbol{r}_n^{(\mathscr{C})}\}_{n=1,\ldots,N}$ can be written as follows: