Exactly solvable problem of nonlinear two-dimensional screening

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An analytic solution is derived for the two-dimensional problem of the nonlinear screening of a system of strong point charges which repel mobile carriers. The problem is reduced to one of determining the shapes of the boundaries of the regions from which the carriers are repelled. It is solved by methods of the theory of functions of a complex variable. The results can be used to calculate the potential of a system of charged dislocations in a semiconductor and for calculations of interactions in such a system.

1. In solid state physics it is often necessary to solve a nonlinear screening equation

$$\Delta\varphi=-4\pi[\rho(\varphi)+\rho_0(\mathbf{r})], \tag{1}$$

where $\rho_0(\mathbf{r})$ is an external charge density, and $\rho(\varphi)$ is an induced charge density. The functional dependence $\rho(\varphi)$ is described by a "jelly" model in which there is a positive smeared background and a mobile electron fluid.

In the linearized formulation of the problem we would have $\rho = -4\pi(\partial\rho/\partial\varphi)_{\varphi=0}\varphi$, and the problem could be solved for an arbitrary function $\rho_0(\mathbf{r})$. The length scale of the screening here is the Debye length $r_D = (-4\pi\partial\rho/\partial\varphi)^{-1/2}$.

If the charges introduced are large enough, the screening becomes nonlinear. In a state of a stable thermodynamic equilibrium, the equation has a unique solution.[1]

If ρ_0 is negative, the screening results from a complete repulsion of electrons from the regions surrounding the charges. In other words, the density $\rho(\varphi)$ is constant within these regions, where it is equal to the charge density of the background; outside these regions, the potential is constant. If the Debye length r_D is much smaller than the size of these regions, we can ignore the variation of the potential ouside such regions. We then would have the following formulation of the problem: We are to find that shape of a region containing a uniformly distributed positive charge and given sources of negative charge which causes the electric field to vanish at the boundary. Since the problem is nonlinear, we cannot use a superposition principle.

The potential distribution becomes independent of the parameters of the electron gas, in particular, the chemical potential and temperature of the gas. Furthermore, this approach turns out to be valid not only for an ideal electron gas but also for a nonideal one, even if it is of a quantum nature, provided that the length scale of the nonlocal coupling of the electron density with the potential is shorter than the size of the space-charge region.

A problem of this form has arisen on several occasions in semiconductor physics. Because of its nonlinearity, however, it has been successfully solved only in very simple cases. In particular, it has been solved in the one-dimensional case for a Schottky layer,[2] in the cylindrically symmetric case for a solitary charged dislocation,[3] and in the spherically symmetric case in a calculation on the optimal fluctuation in a heavily doped semiconductor.[4]

It is found that in the two-dimensional case the problem has several exact solutions. In Ref. 5 we derived a solution for a point source with a potential $\varphi = 2q\ln r + \mathbf{dr}/r^2$ (a rectilinear edge dislocation). In the present paper we find a solution for an arbitrary finite system of point sources

$$\rho_0(\mathbf{r})=\sum_{i=1}^{k} q_i\delta(\mathbf{r}-\mathbf{r}_i).$$

The result reduces to a system of algebraic equations with a number of unknowns equal to twice the number of point sources.

From the formal standpoint this model is suitable for describing the screening of strong point sources in a two-dimensional single-component gas with logarithmic interaction between particles.

A practical example of a system to which the results apply is a set of negatively charged parallel dislocations which are interacting electrostatically with electrons in an n-type semiconductor. Since there is a strain interaction in addition to the electrostatic interaction, the strain interaction must be evaluated. For screw dislocations in an isotropic material, there is no such interaction. For an edge dislocation it is found to be weak under the condition $\Lambda b/2\pi r_0 \ll ne^2/\varepsilon$, where Λ is the strain-energy constant, b is the Burgers vector, n is the linear charge density at the dislocation axis, ε is the dielectric constant, and r_0 is the typical radius of the cylindrical space-charge region around the dislocation axis. In a semiconductor with donors of a single type, this screening model is applicable in the two limiting cases in which the magnitude of the potential in the space-charge region, ne^2/ε, satisfies the conditions $kT \ll ne^2/\varepsilon \ll E_i$ and $ne^2/\varepsilon \gg E_i$, where E_i is the depth of the donor level. In the first case, the screening results from repulsion of mobile electrons, and we therefore have $r_0 = (n/\pi N)^{1/2}$, where N is the density of electrons in the band. In the second case, all the donors are striped, and we have $r_0 = (n/\pi N_i)^{1/2}$, where N_i is the density of donors.

2. We introduce the complex electric field $\mathscr{E} = E_x - iE_y$ and the coordinate $z = x + iy$. The field set up by the point sources and by the uniformally distributed background is described by

$$\mathscr{E}(z)=2\sigma\iint\frac{dS'}{z-z'}-2\sum_{j=1}^{k}\frac{q_j}{z-z_j}, \tag{2}$$

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where the integration is carried out over the area occupied by the background, with a charge density $\sigma > 0$; the z_j are the positions of the charges; and $q_j > 0$. The shape of the region is determined by the condition $\mathscr{E}(z) = 0$ at points z at the boundary of the region. For a fixed integration region, expression (2) determines an analytic continuation of the function $\mathscr{E}(z)$ into the exterior of the space-charge region. If the field $\mathscr{E}$ vanishes at the boundary and at infinity, then it vanished everywhere outside the space-charge region. In the equation determining the boundary of the region $\mathscr{E}(z) = 0$, we can thus assume that z also lies outside the space-charge region everywhere.

Using Stokes' law in complex form, we can transform the area integral in (2) into an integral along the boundary of the region. The equation $\mathscr{E}(z) = 0$ takes the form

$$\frac{\sigma}{2i}\oint_{\Gamma}\frac{dt\bar{t}}{z-t}=\sum_{j=1}^{k}\frac{q_j}{z-z_j}, \tag{3}$$

where $\bar{t}$ is the complex conjugate of t, and the point z is assumed to lie outside the space-charge region. We traverse the boundary Γ in the direction which keeps the corresponding region on our left.

We restrict the discussion to the case of a singly connected space-charge region. We consider the conformal mapping of the region of interest into a unit circle which results from the function $z = \omega(\zeta)$, $|\zeta| \leqslant 1$. We assume that the function $\omega(\zeta)$ is the ratio of two polynomials. In order to use the Cauchy theorem, we need to analytically continue the function $\overline{\omega(\zeta)}$ into the circle. This continuation is carried out by means of the equation $\overline{\omega(\zeta)} = \bar{\omega}(1/\zeta)$, where the function $\bar{\omega}(t)$ differs from $\omega(t)$ in that the coefficients of the polynomials have been replaced by their complex conjugates. The equation for the unknown function $\omega(\zeta)$ becomes

$$\frac{\sigma}{2i}\oint_{|\zeta|=1}\frac{d\zeta\omega'(\zeta)\bar{\omega}(1/\zeta)}{z-\omega(\zeta)}=\sum_{j=1}^{k}\frac{q_j}{z-z_j}. \tag{4}$$

We wish to evaluate the electric field $\mathscr{E}$ in the space-charge region. In order to eliminate the singularity in integral (2), we exclude a small neighborhood of the point z: $|z'-z| \leqslant \delta$. In the limit $\delta \to 0$, the integral over this neighborhood vanishes. The remaining area integral transforms into a sum of contour integrals:

$$\mathscr{E}(z)=\frac{\sigma}{i}\oint_{|\zeta|=1}\frac{d\zeta\omega'(\zeta)\bar{\omega}(1/\zeta)}{z-\omega(\zeta)}-\frac{\sigma}{i}\oint_{|z-t|=\delta}\frac{dt\bar{t}}{z-t}-2\sum_{j=1}^{k}\frac{q_j}{z-z_j}.$$

As a result we find

$$\mathscr{E}(z)=2\pi\sigma[\bar{z}-\bar{\omega}(\zeta^{-1}(z))], \tag{5}$$

where $\zeta(z)$ is a root of the equation $\omega(\zeta) = z$. The potential is given by

$$\varphi=\mathrm{Re}\int_{z}^{\infty}dz\mathscr{E}=2\pi\sigma\left[-|z|^2-\mathrm{Re}\int_{\zeta(z)}^{1}d\eta\omega'(\eta)\bar{\omega}(1/\eta)\right].$$

3. Let us assume that the point $z = 0$ lies inside the space-charge region. We can always arrange this situation by moving the origin of coordinates. The function $\omega(\zeta)$ can then be sought in the form

$$\omega(\zeta)=\zeta\sum_{j=1}^{k}\{c_j/(\zeta-\zeta_j)\} \tag{6}$$

since ω is analytic inside the circle, we have $|\zeta_j| > 1$ for all j. The function $\bar{\omega}(1/\zeta)$ has poles at the points $\zeta = 1/\bar{\zeta}_j$. From Eq. (4) we have the equations

$$\omega(1/\bar{\zeta}_j)=z_j,\quad \omega'(1/\bar{\zeta}_j)\,\mathrm{Res}\,\bar{\omega}(\zeta_j)=q_j/\pi\sigma. \tag{7}$$

From them we finally find the system of equations

$$\sum_{j=1}^{k}\{c_j/(1-\zeta_j\bar{\zeta}_m)\}=z_m,$$

$$\bar{c}_m\bar{\zeta}_m\sum_{j=1}^{k}\{c_j\zeta_j/(1-\zeta_j\bar{\zeta}_m)^2\}=q_m/\pi\sigma, \tag{8}$$

where $m = 1, \ldots, k$. Solving the problem thus reduces to finding the quantities c_j, ζ_j.

The shape of the contour is specified parametrically: $z = \omega(e^{i\varphi})$ for $0 \leqslant \varphi \leqslant 2\pi$. If the contour is to be a boundary, it must not have any self-intersections. This condition filters out some extraneous solutions of system (8), since the solution of the problem is unique.[1,4] It can be seen from (8) that the quantities ζ_j are determined to within a general phase factor $e^{i\vartheta}$, $\vartheta = \text{const}$.

The function (6) maps the point $\zeta = 0$ into $z = 0$. If we do not require the point 0 to remain fixed in the course of the mapping, then we need to add some constant R, which lies inside the space-charge region, to the right side of (6). Correspondingly, we need to subtract R from the right sides of the first of Eqs. (7) or (8).

Adding a constant leaves an invariant region. Specifically, under the linear-fraction transformation

$$\zeta=(w+a)/(1+\bar{a}w),$$

where

$$R=a\sum_{j=1}^{k}\{c_j/(a-\zeta_j)\},\qquad |a|<1,$$

which maps the circle $|\zeta| \leqslant 1$ into the cricle $|w| \leqslant 1$, the arbitrary constant R drops out of Eqs. (6) and (8). The latter take their original form with respect to the renormalized constants c_j and ζ.

Equations (8) do not always have solutions. An absence of solutions is evidence that the region becomes multiply connected. If the space-charge regions breaks up into several singly connected regions (without "holes"), the problem must be solved independently for each of these regions; only those sources which lie inside the corresponding space-charge region are to be taken into consideration. A solution cannot be found in the case of multiply connected regions.

It follows from electrical neutrality that the total area occupied by the space charge is determined by the total charge of the sources and is independent of their positions.

4. As an example we consider the screening of one and two sources. For a charge q at the point z_0 we find

$$\omega(\zeta)=\frac{\zeta}{|z_0|\zeta-r_0}\left(z_0|z_0|-\frac{z_0}{|z_0|}r_0^2\right).$$

The substitution $\zeta = e^{i\varphi}$ determines a circle centered at the point z_0 with a radius $r_0 = (q/\pi\sigma)^{1/2}$. This radius naturally corresponds to the radius for which the total charge in the circle is equal to the charge of the source.

Let us consider the case of two identical sources at the points $x = \pm a/2$ with charges q. If $a > 2r_0$, the region breaks up into two unconnected circles. In the case $a \leqslant 2r_0$ we have

$$z=\omega(\zeta)=2bc\zeta/(\zeta^2-b^2), \quad b=[u+(u^2-1)^{1/2}]^{1/2},$$
$$\mathscr{E}(z)=2\pi\sigma[\bar{z}-2bc\zeta(z)/(1-b^2\zeta^2(z))],$$
$$c=a(u^2-1)^{1/2}/2, \quad u=(2r_0/a)^2. \tag{9}$$

The region determined by (9) is dumbbell-shaped.

Using expression (9) for $\mathscr{E}$, we can find the force of the electrostatic interaction of two charged dislocations separated by a distance $a \leqslant 2r_0$ (at greater distances, the dislocations do not interact at all). Calculating the field near the point $z = a/2$, we find the force to be

$$|F| = \frac{\pi}{2}\sigma a q(u-1)[u+1-(u^2-1)^{1/2}].$$

The repulsive force decreases to zero in proportion to $a - 2r_0$ in the limit $a \to 2r_0$.

5. Let us assume that a small test charge is added to the system in the space-charge region. The potential produced by this test charge can be found by assuming that the boundary of the region is fixed, and that the boundary condition $\varphi = 0$ holds on it. These assumptions mean that the boundary is acting as a grounded metal electrode.[6] The reason is that the electron density is so high that the Debye length is shorter than all the length scales in the system.

To prove this assertion, we set the field variation $\delta\mathscr{E}(z)$ caused by the insertion of a test charge δq equal to zero at all points outside the space-charge region:

$$2\sigma \iint \frac{d\delta S'}{z-z'} + \frac{2\delta q}{z-z_0} = 0. \tag{10}$$

If we transform the area integral into a contour integral by means of the substitution $d\delta S = dl dh$, where dh is the deviation of a point of the contour along the normal, and dl is an element of length along the boundary, we find that the latter equation is the same as the equation for the surface charge density $\sigma\delta h$ on a grounded metal electrode with shape corresponding to the unperturbed contour.

If the problem with initial charges has been solved, so that the function $\omega(\zeta)$ which maps the boundary of the region into a circle, has been found, the solution of the perturbed problem can be expressed directly in terms of this function: $\varphi(\zeta) = 2\delta q \ln|(1-\zeta\bar{\zeta}_0)/(\zeta-\bar{\zeta}_0)|$, where $\omega(\zeta) = z$.

6. In a problem with a finite number of sources, a complete (not exponential) screening of the field occurs at large distances. What happens if point sources are distributed with a given density c over the entire plane? If the density is low, $\pi c r_0^2 \ll 1$, space-charge regions usually surround isolated point charges or small groups of charges. The shapes of the regions can be calculated without consideration of the other charges. The screening remains complete. If the density is high, $\pi c r_0^2 \sim B_c$, an infinite cluster of electrically neutral regions disappears.

Above the percolation threshold, the system constitutes a set of uncoupled neutral regions, so the the field of a test charge extends over arbitrarily large distances, falling off exponentially with distance. At the point of the percolation transition the complete screening gives way to exponential screening at large distances. This change apparently implies a corresponding behavior of the potential correlation at large distances.

The method developed in this study can be used to solve other problems involving nonlinear screening. In particular, it is possible to find the potential set up by a system of uniformly charged straight line segments positioned on a common line or that set up by a corresponding system of metal electrodes with given potentials.

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