Sheath above an electron emitting surface

Consider two parallel plates in vacuum and assume that one is illuminated by ultraviolet light (UV) and emits photoelectrons. There will be a cloud of photoelectrons between the plates and the electrostatic potential $\phi$ between the plates will be negative. We will assume that the potential at each plate is specified and then we will solve for the potential $\phi(x)$ with the specified boundary conditions. The problem is assumed one-dimensional. We do not need to solve the equations of motion for the electrons. Instead, we will assume that a one-sided Maxwellian distribution of electrons is emitted at the left boundary and use kinetic theory to find the distribution and the electron density at points between the plates.

The method for solving the problem will be broken into two parts: (1) the procedure for solving Poisson's equation and (2) the procedure for finding the electron density from $f(v)$ using kinetic theory. The sheath potential $\phi(x)$ is nonmonotonic which requires that we use different expressions for the electron density to the left and to the right of the potential minimum.

Method for solving Poisson's equation

Poisson's equation will be solved by successive approximations using the finite-differencing method introduced in the exercise "Poisson's Equation and Debye Shielding." The starting point is Poisson's equation:

$$- \frac{d^2}{dx^2} \Phi(x) = \left[ n_i(x) - n_e(x) \right] \frac{q}{\varepsilon_0}$$

In finite-difference form, the second derivative is

$$\frac{d^2\Phi}{dx^2} = \frac{1}{\Delta x^2} \left[ \Phi_{k+1} - 2\Phi_k + \Phi_{k-1} \right]$$

where $x_k$ is the $k$th grid point, $\Delta x$ is the grid point spacing, and $\Phi_k = \phi(x_k)$.

Poisson's equation can be rewritten as

$$\Phi_k \leftarrow \frac{1}{2} \left[ \Phi_{k+1} + \Phi_{k-1} \right] + \frac{1}{2} (\Delta x)^2 \left[ n_i(x_k) - n_e(x_k) \right] q / \varepsilon_0$$

The left arrow indicates that the present value of $\phi(x_k)$ is to be replaced by the value on the right hand side. This procedure is repeated until the solution for $\Phi$ has "relaxed" to a final value. The densities of electrons and ions are found as a function of the potential $\phi(x_k)$. An initial guess is used for $\phi(x_k)$ in the first iteration.

Method for finding the electron density

The emitted distribution of electrons will be assumed to be a single-sided Maxwellian for simplicity. If the UV passes through a window in an experiment, the UV spectrum will be cut off at the shortest wavelengths because of absorption by the window material. Thus there will be an upper bound on the energy of the UV photons and this results in an upper bound on the energy of the photoelectrons. This upper bound is ignored in our analysis. If the electrons are from thermionic emission from a heated surface rather than from photoemission, there is no need to assume a cutoff.
The anticipated solution for $\Phi(x)$ is sketched at right. The potential has a minimum $\Phi_{\text{min}}$ that is nearer to the photoemitting plate than to the other plate. Electrons emitted at $x = 0$ with energy less than $-q\Phi_{\text{min}}$ are reflected by the potential and return to $x = 0$. The electrons with more energy pass over the potential "hill" for electrons and are absorbed at $x = L$. Thus electrons with energy less than $-q\Phi_{\text{min}}$ contribute twice to the density to the left of the minimum, once leaving and once returning. The location of the minimum is $x_{\text{min}}$.

The one-sided Maxwellian with density $n_0$ is

$$f(v, \Phi) = n_0 \left( \frac{m_e}{2\pi T_e} \right)^{1/2} \exp \left( \frac{q\Phi - m_e v^2}{2T_e} \right)$$

where $T_e$ is the electron temperature, $q$ is the electron charge, $m_e$ is the electron mass, and $n_0$ is the density if $v$ is both positive and negative.

The exponential part is

$$\exp \left( -\frac{W}{T_e} \right) \quad \text{with} \quad W = -q\Phi + \frac{1}{2} m_e v^2$$

The total energy $W$ is a constant of the motion, thus $f(v, \Phi)$ is constant along a trajectory and applies at all points in the region that particles can reach. If $\Phi$ is zero everywhere, the density can be found at any point by integrating $f(v)$ over all velocities. However, in the presence of the potential minimum, electrons that do not make it over the top of the potential hill in energy are not present for $x > x_{\text{min}}$ and in this region the integral must be started at some minimum velocity.

It is useful to switch to a dimensionless system of units. In the second line at right we have multiplied or divided all the terms in Poisson's equation (the first line) by constants so that the last two bracketed terms are dimensionless. We then recognize that the first bracketed term is the Debye length squared and that this length is used to make the $x$ derivatives dimensionless as well. The last four lines show the dimensionless versions of the variables.

$$- \frac{d^2}{dx^2} \Phi(x) = \left( n_i(x) - n_e(x) \right) q / \varepsilon_0$$

$$- \left( \frac{\varepsilon_0 T_e}{n_0 q^2} \right) \frac{d^2}{dx^2} \left( \frac{q\Phi(x)}{T_e} \right) = \left( n_i(x) - n_e(x) \right) / n_0$$

$$\frac{d^2}{dx^2} \tilde{\Phi}(\tilde{x}) = \tilde{n}_i(\tilde{x}) - \tilde{n}_e(\tilde{x})$$

$$\tilde{\Phi} = q\Phi / T_e$$

$$\tilde{x} = \frac{x}{\sqrt{\varepsilon_0 T_e / n_0 q^2}} = \frac{x}{\lambda_{\text{Debye}}}$$

$$\tilde{n} = n / n_0$$

$$\tilde{v} = \frac{v}{\sqrt{2T_e / m_e}}$$

In the pages below, we will use dimensionless variables and omit the tildes.
We now define a Maxwellian in the dimensionless system (omitting the tildes):

\[ f(v, \phi) := \frac{1}{\sqrt{\pi}} \exp\left(\frac{\phi - v^2}{2}\right) \int_{-\infty}^{\infty} f(v, 0) \, dv = 1 \]

**Density \( n_1 \) in the region \( x < x_{\text{min}} \)**

At the origin, electrons with energy less than \(-\phi_{\text{min}}\) (in the dimensionless units) are reflected and count twice toward the density. To the right of the origin, electrons that are reflected that locally have \( v^2 - \phi > -\phi_{\text{min}} \), hence electrons with \( v^2 > (\phi - \phi_{\text{min}}) \) pass through this region going to the right and do not return, thus they count only once. The density for \( x < x_{\text{min}} \) is then found by integrating \( f(v) \) over all positive velocities (emitted electrons going to the right) and over negative velocities corresponding to the particles reflected. The reflected particles have \( v^2 < (\phi - \phi_{\text{min}}) \).

\[ n_1(\phi, \phi_{\text{min}}) := \int_{0}^{\infty} f(v, \phi) \, dv + \int_{-\sqrt{\phi - \phi_{\text{min}}}}^{0} f(v, \phi) \, dv \]

In this definition, \( \phi \) is a dummy variable that is the argument of the density function.

\[ n_1(\phi, \phi_{\text{min}}) := 0.5 \exp(\phi) \cdot \left( 1 + \text{erf}\left(\sqrt{\phi - \phi_{\text{min}}}\right) \right) \]

The integrals above have solutions in terms of known functions.

We can check the normalization by noting that the density should approach unity if \( \phi_{\text{min}} \) is so negative that all particles are reflected. Thus we let \( \phi = 0 \) (the left boundary condition) and let \( \phi_{\text{min}} = -4 \), and get

\[ n_1(0, -4) = 0.998 \]

This value approaches unity (as it should) as \( \phi_{\text{min}} \) becomes more negative.

**Density \( n_2 \) in the region \( x > x_{\text{min}} \)**

For \( x > x_{\text{min}} \), the density integral includes only positive velocities that have passed over the barrier

\[ n_2(\phi, \phi_{\text{min}}) := \int_{\sqrt{\phi - \phi_{\text{min}}}}^{\infty} f(v, \phi) \, dv \]

\[ n_2(\phi, \phi_{\text{min}}) := 0.5 \exp(\phi) \cdot \text{erfc}\left(\sqrt{\phi - \phi_{\text{min}}}\right) \]

The integral has solutions in terms of known functions.

We can check this by noting that the density should be 0.5 if \( \phi_{\text{min}} = 0 \) and no particles are reflected:

\[ n_2(0, 0) = 0.5 \]
The two expressions for the density agree at the top of a potential hill, where the regions meet:

\[ n_1(-1, -1) = 0.184 \quad n_2(-1, -1) = 0.184 \]

The density is a continuous function.

**Try it:** Explore the behavior of \( n_1 \) and \( n_2 \) for other values of \( \Phi \) and \( \Phi_{\text{min}} \).

**Define the x grid**

\( \Delta x \) will be the grid spacing. Stability requires that we make this small enough to resolve details on the scale of the Debye length, so we will make \( \Delta x = 0.5 \) because the Debye length will be unity if all electrons are reflected. A vector (a matrix with one row) will contain the values of \( \Phi_k \).

- \( k_{\text{max}} := 40 \) There will be \( k_{\text{max}}+1 \) grid points.
- \( \Delta x := 0.5 \) Grid spacing in Debye lengths.
- \( k := 0, 1 \ldots k_{\text{max}} \)
- \( x_k := k \cdot \Delta x \)
- \( x_{k_{\text{max}}} = 20 \) These grid points define a domain that is 20 Debye lengths long.

**The trial solution for the first iteration**

Our initial guess for the answer will be an inverted parabola with a minimum at -1.

\[ \Phi_{\text{Guess}}_k := 4 \left( \frac{0.5 \cdot x_{k_{\text{max}}} - x_k}{x_{k_{\text{max}}}} \right)^2 - 1 \]

At right is a plot of the initial guess.

In our program loop we will need to find the location \( x_{\text{min}} \) of the minimum in the potential. This will be done using the \texttt{min} function to first find \( \Phi_{\text{min}} \). The method will be tested using \( \Phi_{\text{Guess}} \).

\[ \text{phimin := min(PhiGuess)} \quad \text{phimin = -1} \]

The lookup function is now used to find the value of \( x \) corresponding to \( \text{phimin} \):

\[ x_{\text{min}} := \text{lookup(phimin, PhiGuess, x)}_0 \]

\[ x_{\text{min}} = 10 \]

The subscript zero is used to return the first minimum that is found, in case there are several points with the same potential value \( \text{phimin} \).
In our program loop, the $i$th iteration finds the new $\Phi$ values from the $(i-1)$th iteration which is in column $i-1$ of the temporary answer matrix $\Phi$. Thus we will need to find the minimum value of $\Phi$ in the $i-1$ column of $\Phi$. The program loop lines to find $x_{\text{min}}$ are

$$\text{phimin} \leftarrow \min(\Phi^{(i-1)})$$

$$x_{\text{min}} \leftarrow \text{lookup}(\text{phimin}, \Phi^{(i-1)}, x)_0$$

### Solution to Poisson's equation by successive approximations

The $\Phi$ values are saved in a temporary (local) matrix $\Phi$. Each row in the matrix will be an iteration.

\[ \text{iters} := 4 \cdot \text{ceil} \left( \frac{x_{\text{max}}^2}{2} \right) \quad \text{iters} = 1.6 \times 10^3 \]

The number of iterations. The plot below requires that iters be divisible by 4.

The problem we are solving is similar to a diffusion problem. A good guess for the "relaxation time" is the square of the maximum value of $x$ because diffusion times scale as the square of the length. We will use 4 "relaxation times" to be sure of convergence.

The following if statement is used to select $n_1$ for the density if $x < x_{\text{min}}$ and $n_2$ for the density otherwise.

\[ n_e \leftarrow \text{if}(x_k < x_{\text{min}}, n_1(\Phi^{(i-1)}, \text{phimin}), n_2(\Phi^{(i-1)}, \text{phimin})) \]

The program loop below begins by placing the initial guess in the first column of the answer matrix $\Phi$.

\[
\Phi(\Phi\text{Guess}) :=
\begin{align*}
\Phi_{\text{max}, \text{iters}} & \leftarrow 0 \\
\Phi^{(0)} & \leftarrow \Phi\text{Guess} \\
\Phi\text{New}_{\text{max}} & \leftarrow 0 \\
\text{for} \quad i \in 1 \ldots \text{iters} \\
\quad \text{phimin} & \leftarrow \min(\Phi^{(i-1)}) \\
\quad x_{\text{min}} & \leftarrow \text{lookup}(\text{phimin}, \Phi^{(i-1)}, x)_0 \\
\quad \text{for} \quad k \in 1 \ldots \text{kmax} - 1 \\
\quad \quad n_e & \leftarrow \text{if}(x_k < x_{\text{min}}, n_1(\Phi^{(i-1)}, \text{phimin}), n_2(\Phi^{(i-1)}, \text{phimin})) \\
\quad \quad \Phi\text{New}_k & \leftarrow 0.5 \left( \Phi^{(i-1)}_{k+1} + \Phi^{(i-1)}_{k-1} \right) + 0.5 \cdot \Delta x^2 \cdot (-n_e) \\
\quad \quad \Phi^{(i)} & \leftarrow 0.5 \left( \Phi\text{New} + \Phi^{(i-1)} \right) \\
\quad \quad \Phi^{(i)}_{\text{max}} & \leftarrow \left( \Phi^{(i-1)} \right)_{\text{max}} \\
\quad \quad \left( \Phi^{(i)} \right)_0 & \leftarrow \left( \Phi^{(i-1)} \right)_0 \\
\end{align*}
\]

\[ \Phi \]
The last two lines in the "for i" loop preserve the boundary conditions at \( k = 0 \) and \( k = k_{max} \).
The iterative technique is stable if the new answer \( \Phi_{\text{New}} \) is averaged with the old answer before it is used. The averaging is at the end of the "for k" loop. This averaging is discussed in the exercise "Poisson's Equation and Debye Shielding."

The program loop above is written as a function of \( \Phi_{\text{Guess}} \) so that we can use a different \( \Phi_{\text{Guess}} \) later and not have to write out the program loop again. We will place the answer in a new matrix \( \Phi \) so that we don't have to evaluate the function \( \Phi(\Phi_{\text{Guess}}) \) every time that we need to use \( \Phi \).

\[
\Phi := \Phi(\Phi_{\text{Guess}})
\]

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This plot shows several of the successive approximation to the potential between the plates:
The photoelectrons are emitted on the left thus the sheath forms nearer the left boundary.

**Try it:** Find a solution with a poor initial guess, such as zeroes everywhere. Does a poor initial guess change the answer?

**Test for convergence**

Did we use a large enough value for iters to converge to the correct answer? We can answer this question by watching the evolution of Phimin.

\[ i := 0 \ldots \text{iters} \]
\[ \text{Phimin}_i := \min\left(\Phi^{(j)}\right) \]

The vector Phimin contains the successive values of the minimum in \( \Phi \).

A plot of the values of Phimin that show convergence toward an answer:

![Plot of Phimin](image)

This plot shows that our initial guess for the number of iterations iters was a good one.

**Plot of number density**

The number density is a complicated function of the potential. Recall that in our program loop:

\[ n_e \leftarrow \text{if } x_k < \text{xmin}, n_1\left(\left(\Phi^{(j-1)}\right)_k, \text{phimin}\right), n_2\left(\left(\Phi^{(j-1)}\right)_k, \text{phimin}\right) \]

To use this definition outside the loop we will put the final column of the matrix Phi into a vector PhiFinal:

\[ \text{PhiFinal} := \Phi^{(\text{iters})} \]
\[ \text{phimin} := \min(\text{PhiFinal}) \]
\[ \text{phimin} = -2.393 \]
\[ \text{xmin} := \text{lookup(phimin, PhiFinal, x)} \]
\[ \text{xmin} = 7 \]

\[ N_e_k := \text{if } x_k < \text{xmin}, n_1\left(\text{PhiFinal}_k, \text{phimin}\right), n_2\left(\text{PhiFinal}_k, \text{phimin}\right) \]
Linear plot and log plot of the electron density

The electron density drops sharply at the emitting surface.

Solution with a new set of boundary conditions

Suppose we place a negative bias of $-1.8$ on the right hand boundary. This will cause more of the electrons to be reflected. Will there still be a minimum between the boundaries?

What should we use for an initial guess for $\Phi_k$? We saw above that a good initial guess is not essential. The easiest thing to do is to have all the $\Phi$ values zero except for the right boundary which will be set to $-1.8$.

\[
\text{PhiGuess}_k := 0 \quad \text{PhiGuess}_{k_{\text{max}}} := -4
\]

Find the answer: \[
\Phi := \Phi(\text{PhiGuess}) \quad \text{Put it in PhiFinal3:} \quad \text{PhiFinal3} := \Phi^{\langle \text{iters} \rangle}
\]
The plot above shows that for this choice for the potential on the right boundary, the potential falls most strongly in the sheath region and is more nearly constant outside the sheath.

**Try it:** What does the plot of density look like for this case?

**Try it:** Change the right boundary potential to $-2.5$. Is there a minimum in the potential? How about for $-3$?

**Try it:** The number of iterations iters is calculated from the size of the domain. If kmax is changed from 40 to 80 so that there are 40 Debye lengths in the domain, then the number of iterations is automatically increased by a factor of four. Is the convergence as good if kmax = 80? Does the method for calculating iters seem to be correct?

**References**