# Notes on Vacuum Electronics Molecular Dynamics Simulations

Kristinn Torfason

January 19, 2018

# 1 Verlet Integration

$$\mathbf{x}_{n+1} = 2\mathbf{x}_n - \mathbf{x}_{n-1} + \frac{\mathbf{F}_n(\mathbf{x}_n)}{m}\Delta t^2 \tag{1}$$

Force on a particle at $\mathbf{r}$ due to all other particles at positions $\mathbf{r}_i$

$$\mathbf{F}(\mathbf{r}) = \frac{q^2}{4\pi\varepsilon_0}\sum_{i=1}^{N}\frac{\mathbf{r} - \mathbf{r}_i}{|\mathbf{r} - \mathbf{r}_i|^3} \tag{2}$$

Force on a particle due to an electric field drgdrterter

$$F(\mathbf{r}) = qE(\mathbf{r}) \tag{3}$$

in case of a constant field in the $z$-direction $\mathbf{E} = [0, 0, E_z]$

$$F_z = qE_z = q\frac{V}{d}, \tag{4}$$

where $V$ is the voltage and $d$ the gap distance. Initial fictitious previous position

$$x_{n-1} = x_n - v_0\Delta t - \frac{F(x_n)}{2m}\Delta t^2 \tag{5}$$

where $v_0$ is the initial velocity.

## 1.1 Velocity Verlet

The Velocity Verlet method is done in three steps, fyrst update the position,

$$x_{n+1} = x_n + v_n\Delta t + \frac{1}{2}a_n\Delta t^2, \tag{6}$$

then calculate the acceleration $a_{n+1}$ using $x_{n+1}$ and finaly update the velocity,

$$v_{n+1} = v_n\frac{a_n + a_{n+1}}{2}\Delta t^2. \tag{7}$$

Note this method assumes that $a_{n+1}$ dose not depend on $v_{n+1}$. This could be a problem when using a magnetic field which depends on the velocity. First approximation would be to use $v_n$ if the field is week, see also [4].

### 1.1.1 Nondimensionalization

Set $x_n = L\bar{x}_n$, where $L$ is a characteristics length scale and $\bar{x}_n$ is a dimensionless length. Similarly set $v_n = T\bar{v}_n$ where $T$ is a characteristics time scale for the system. Then $\Delta t = T\Delta\bar{t}$ and $a_n = \frac{L}{T^2}\bar{a}_n$. The equations then become,

$$\bar{x}_{n+1} = \bar{x}_n + \bar{v}_n\Delta\bar{t} + \frac{1}{2}\bar{a}_n\Delta\bar{t}^2, \tag{8}$$

and,

$$\bar{v}_{n+1} = \bar{v}_n\frac{\bar{a}_n + \bar{a}_{n+1}}{2}\Delta\bar{t}^2. \tag{9}$$

In program $L = 1.0 * 10^{-9}$ m and $T = 1.0 * 10^{-12}$ s, i.e. lengths are scaled in nanometers and time in pico-seconds.

For the Coulomb force we have,

$$F_1 = \frac{q_1 q_2}{4\pi\epsilon} \frac{x_1 - x_2}{|x_1 - x_2|^3} \,. \tag{10}$$

Setting $x = L\bar{x}$ gives

$$F_1 = \frac{q_1 q_2}{4\pi\epsilon} \frac{1}{L^2} \frac{\bar{x}_1 - \bar{x}_2}{|\bar{x}_1 - \bar{x}_2|^3} \,. \tag{11}$$

We wish to find the acceleration using $F = ma = m\frac{L}{T^2}\bar{a}$ or

$$\bar{a}_1 = \frac{q_1 q_2}{4\pi m\epsilon} \frac{T^2}{L^3} \frac{\bar{x}_1 - \bar{x}_2}{|\bar{x}_1 - \bar{x}_2|^3} \,. \tag{12}$$

The acceleration from the electric field in the system is given by,

$$F = qE = q\frac{V}{d} \,, \tag{13}$$

where $d$ is the gap spacing and $V$ the voltage over the gap. We set $d = L\bar{d}$ and $F = m\frac{L}{T^2}$ and obtain,

$$\bar{a} = \frac{qV}{m\bar{d}} \frac{T^2}{L^2} \,. \tag{14}$$

## 1.2  Unit Test Case

Two electrons and one hole.
Fyrst electron: $x_1 = 3\,\mathrm{nm}$, $y_1 = -10\,\mathrm{nm}$, $z_1 = 101\,\mathrm{nm}$.
Second electron: $x_2 = -9\,\mathrm{nm}$, $y_2 = 26\,\mathrm{nm}$, $z_2 = 80\,\mathrm{nm}$.
The hole: $x_3 = 6\,\mathrm{nm}$, $y_3 = -24\,\mathrm{nm}$, $z_3 = 118\,\mathrm{nm}$.
Parameters: $d = 100\,\mathrm{nm}$, $V = 2\,\mathrm{V}$, $\Delta t = 0.25\,\mathrm{ps}$.
   The acceleration of the fyrst electron is

$$\mathbf{a}_{12} = \frac{e^2}{4\pi m\epsilon_0} \frac{\mathbf{R}_1 - \mathbf{R}_2}{|\mathbf{R}_1 - \mathbf{R}_2|^3} \tag{15}$$

$$\mathbf{a}_{13} = -\frac{e^2}{4\pi m\epsilon_0} \frac{\mathbf{R}_1 - \mathbf{R}_3}{|\mathbf{R}_1 - \mathbf{R}_3|^3} \tag{16}$$

# 2 Field Emission

## 2.1 Fowler-Nordheim equation

$$J = \frac{a}{\phi t^2(l)} F^2 exp(-\nu(l) b \phi^{3/2}/F) \tag{17}$$

where $a \approx 1.541434 \times 10^{-6}\,\mathrm{AeVV^{-2}}$ and $b \approx 6.830890\,\mathrm{eV^{-3/2}Vnm^{-1}}$ are the first and second Fowler-Nordheim constants (see equation (22) and (23)).

The equation for $\nu(l)$ is [1]

$$\nu(l) = 1 - l + \frac{1}{6} l\,ln(l) \tag{18}$$

and for $t(l)$

$$t(l) = 1 + l \left( \frac{1}{9} - \frac{1}{18}\,ln(l) \right) \tag{19}$$

where

$$l = \frac{F}{F_\phi} = \frac{e^3}{4\pi\epsilon_0} \frac{F}{\phi^2} \tag{20}$$

If $\phi$ is in eV and $F$ in V/m then

$$l = \frac{e}{4\pi\epsilon_0} \frac{F}{\phi^2} \tag{21}$$

The first Fowler-Nordheim constant is in SI units

$$a_{FN} = \frac{e^3}{8\pi h} \tag{22}$$

and has units $\mathrm{AJV^{-2}}$. If we convert to $\mathrm{AeVV^{-2}}$ then we must multiply with $1/e$ to obtain

$$a_{FN} = \frac{e^2}{8\pi h} = \frac{e^2}{16\pi^2\hbar} \tag{23}$$

The second Fowler-Nordheim constant is in SI units

$$b_{FN} = \frac{8\pi}{3eh} \sqrt{2m_e} \tag{24}$$

and has the units $\mathrm{J^{-3/2}Vm^{-1}}$. If we convert it to $\mathrm{eV^{-3/2}Vm^{-1}}$ then we must multiply it with a factor of $(1/e)^{-3/2}$ and obtain

$$b_{FN} = \frac{8\pi\sqrt{2m_e e}}{3h} = \frac{4}{3\hbar} \sqrt{2em_e} \tag{25}$$

## 2.2 Surface Field Calculations

If we assume a box with height $d$ in $z$, length $L$ in $x$ and $y$, with a charge density $\sigma(z)$. Then the surface field at the middle of the bottom in the $z$ direction is given by

$$E = E_0 + 2 \int_0^d \int_{-\frac{L}{2}}^{\frac{L}{2}} \int_{-\frac{L}{2}}^{\frac{L}{2}} \frac{1}{4\pi\epsilon_0} \frac{z\sigma(z)}{(x^2 + y^2 + z^2)^{3/2}}\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,. \tag{26}$$

The factor of two before the integral is to account for image charge effects. If all lengths are scaled with the gap spacing $d$, $\hat{x} = x/d$, $\hat{y} = y/d$ and $\hat{z} = z/d$. Charge density scaled with $\sigma_0 = 4\pi V_0 \epsilon_0 / d^2$, which leads to that current density is scaled by the Child Langmuire limit $\hat{J} = J/J_{CL}$, or $\hat{\sigma}(\hat{z}) = \hat{J}/9\pi\sqrt{\hat{z}}$. The field is scaled by the vacuum field $E_0 = -V_0/d$, we then obtain

$$E = 1 - \frac{2J}{9\pi} \int\limits_{0}^{1} \int\limits_{-\frac{L}{2d}}^{\frac{L}{2d}} \int\limits_{-\frac{L}{2d}}^{\frac{L}{2d}} \frac{\sqrt{\hat{z}}}{(\hat{x}^2 + \hat{y}^2 + \hat{z}^2)^{3/2}} \, \mathrm{d}\hat{x} \, \mathrm{d}\hat{y} \, \mathrm{d}\hat{z} \,. \tag{27}$$

Calculated iteratively

## 2.3 Prolate spheroidal coordinates

The prolate spheroidal coordinates are defined as

$$\begin{aligned} x &= a \sinh \mu \sin \nu \cos \phi \\ y &= a \sinh \mu \sin \nu \sin \phi \\ z &= a \cosh \mu \cos \nu \end{aligned} \tag{28}$$

Set $\xi = \cosh \mu$ and $\eta = \cos \nu$ then

$$\begin{aligned} \sinh^2 \mu &= \cosh^2 \mu - 1 = \xi^2 - 1 \\ \sin^2 \nu &= 1 - \cos^2 \nu = 1 - \eta^2 \end{aligned} \tag{29}$$

which gives

$$\begin{aligned} x &= a\sqrt{\xi^2 - 1}\sqrt{1 - \eta^2} \cos \phi \\ y &= a\sqrt{\xi^2 - 1}\sqrt{1 - \eta^2} \sin \phi \\ z &= a\xi\eta \end{aligned} \tag{30}$$

The reverse are

$$\begin{aligned} \xi &= \frac{1}{2a} \left( \sqrt{x^2 + y^2 + (z + a)^2} + \sqrt{x^2 + y^2 + (z - a)^2} \right) \\ \eta &= \frac{1}{2a} \left( \sqrt{x^2 + y^2 + (z + a)^2} - \sqrt{x^2 + y^2 + (z - a)^2} \right) \\ \phi &= \arctan \frac{y}{x} \end{aligned} \tag{31}$$

To find $\xi$ or $z$ if given $x$ and $y$

$$\xi = \frac{1}{a\sqrt{1 - \eta^2}} \sqrt{x^2 + y^2 + a^2(1 - \eta^2)} \tag{32}$$

$$z = \frac{\eta}{\sqrt{1 - \eta^2}} \sqrt{x^2 + y^2 + a^2(1 - \eta^2)} \tag{33}$$

Derivatives of the coordinates

$$\frac{\partial x}{\partial \xi} = a\xi \frac{\sqrt{1-\eta^2}}{\sqrt{\xi^2-1}} \cos\phi, \quad \frac{\partial y}{\partial \xi} = a\xi \frac{\sqrt{1-\eta^2}}{\sqrt{\xi^2-1}} \sin\phi, \quad \frac{\partial z}{\partial \xi} = a\eta,$$

$$\frac{\partial x}{\partial \eta} = -a\eta \frac{\sqrt{\xi^2-1}}{\sqrt{1-\eta^2}} \cos\phi, \quad \frac{\partial y}{\partial \eta} = -a\eta \frac{\sqrt{\xi^2-1}}{\sqrt{1-\eta^2}} \sin\phi, \quad \frac{\partial z}{\partial \eta} = a\xi,$$

$$\frac{\partial x}{\partial \phi} = -a\sqrt{\xi^2-1}\sqrt{1-\eta^2} \sin\phi, \quad \frac{\partial y}{\partial \phi} = a\sqrt{\xi^2-1}\sqrt{1-\eta^2} \cos\phi, \quad \frac{\partial z}{\partial \phi} = 0.$$

$$(34)$$

The gradient is

$$
\begin{aligned}
\nabla V(\xi,\eta,\phi) &= \hat{x}\frac{\partial V}{\partial x} + \hat{y}\frac{\partial V}{\partial y} + \hat{z}\frac{\partial V}{\partial z} \\
&= \hat{x}\left(\frac{\partial V}{\partial \xi}\frac{\partial \xi}{x} + \frac{\partial V}{\partial \eta}\frac{\partial \eta}{x} + \frac{\partial V}{\partial \phi}\frac{\partial \phi}{x}\right) \\
&+ \hat{y}\left(\frac{\partial V}{\partial \xi}\frac{\partial \xi}{y} + \frac{\partial V}{\partial \eta}\frac{\partial \eta}{y} + \frac{\partial V}{\partial \phi}\frac{\partial \phi}{y}\right) \\
&+ \hat{z}\left(\frac{\partial V}{\partial \xi}\frac{\partial \xi}{z} + \frac{\partial V}{\partial \eta}\frac{\partial \eta}{z} + \frac{\partial V}{\partial \phi}\frac{\partial \phi}{z}\right)
\end{aligned}
$$

$$(35)$$

The position vector is

$$\vec{r} = \begin{pmatrix} a\sqrt{(\xi^2-1)(1-\eta^2)} \cos\phi \\ a\sqrt{(\xi^2-1)(1-\eta^2)} \sin\phi \\ a\xi\eta \end{pmatrix}, \tag{36}$$

and the unit vector are then

$$\hat{\xi} = \frac{\frac{\mathrm{d}\vec{r}}{\mathrm{d}\xi}}{\left|\frac{\mathrm{d}\vec{r}}{\mathrm{d}\xi}\right|}, \quad \hat{\eta} = \frac{\frac{\mathrm{d}\vec{r}}{\mathrm{d}\eta}}{\left|\frac{\mathrm{d}\vec{r}}{\mathrm{d}\eta}\right|}, \quad \hat{\phi} = \frac{\frac{\mathrm{d}\vec{r}}{\mathrm{d}\phi}}{\left|\frac{\mathrm{d}\vec{r}}{\mathrm{d}\phi}\right|}. \tag{37}$$

For $\hat{\eta}$ we have

$$\hat{\eta} = \sqrt{\frac{1-\eta^2}{\xi^2-\eta^2}} \begin{pmatrix} -\eta\sqrt{\frac{\xi^2-1}{1-\eta^2}} \cos\phi \\ -\eta\sqrt{\frac{\xi^2-1}{1-\eta^2}} \sin\phi \\ \xi \end{pmatrix} \tag{38}$$

Scale factors are

$$h_\xi = a\sqrt{\frac{\xi^2-\eta^2}{\xi^2-1}}, \quad h_\eta = a\sqrt{\frac{\xi^2-\eta^2}{1-\eta^2}}, \quad h_\phi = a\sqrt{(\xi^2-1)(1-\eta^2)} \tag{39}$$

Given $x$, $y$ and $\eta_1$

$$\xi = \frac{1}{a}\frac{1}{\sqrt{1-\eta_1^2}}\sqrt{x^2+y^2+a^2(1-\eta_1^2)} \tag{40}$$

### 2.3.1 Electric Field for Hyperbolid Tip

The vector potential is [2]

$$V(\eta) = V_0 \frac{ln\left[\frac{1+\eta_1}{1-\eta_1}\frac{1-\eta}{1+\eta}\right]}{ln\left[\frac{1+\eta_1}{1-\eta_1}\frac{1-\eta_2}{1+\eta_2}\right]}. \tag{41}$$

The boundary conditions have been swaped from Ref. [2]. The tip is now held at $V = 0$ and the anode at $V = V_0$. The derivative of the potential is

$$\frac{dV(\eta)}{d\eta} = -\frac{2V_0}{1-\eta^2}ln^{-1}\left[\frac{1+\eta_1}{1-\eta_1}\frac{1-\eta_2}{1+\eta_2}\right] \tag{42}$$

The gradient in Prolate-Spherodial coordinates is

$$\nabla V(\eta) = \frac{1}{a}\sqrt{\frac{1-\eta^2}{\xi^2-\eta^2}}\frac{dV(\eta)}{d\eta}\hat{\eta}, \tag{43}$$

and the electric field is

$$\vec{E} = -\nabla V(\eta) = \frac{2V_0}{a}\frac{1}{\xi^2-\eta^2}\frac{1}{ln\left[\frac{1+\eta_1}{1-\eta_1}\frac{1-\eta_2}{1+\eta_2}\right]}\begin{pmatrix} -\eta\sqrt{\frac{\xi^2-1}{1-\eta^2}}\cos\phi \\ -\eta\sqrt{\frac{\xi^2-1}{1-\eta^2}}\sin\phi \\ \xi \end{pmatrix} \tag{44}$$

Here $\xi$, $\eta$ and $\phi$ are the position inside the diode. While $\eta_1$ is the hyberbolid tip and $\eta_2 = 0$ is the anode plane.

$$|\vec{E}| = \frac{2V_0}{a}\frac{1}{\sqrt{\xi^2-\eta^2}\sqrt{1-\eta^2}}\frac{1}{ln\left[\frac{1+\eta_1}{1-\eta_1}\frac{1-\eta_2}{1+\eta_2}\right]} \tag{45}$$

At the top of the tip we have $\eta = \eta_1$ and $\xi = 1$ and the electric field points in the $z$-direction,

$$E_z = \frac{2V_0}{a}\frac{1}{1-\eta_1^2}\frac{1}{ln\left[\frac{1+\eta_1}{1-\eta_1}\right]}. \tag{46}$$

### 2.3.2 Area Calculations for Hyperbolid Tip

The Surface area is given by the integral

$$A = \int_{\xi_1}^{\xi_2}\int_{\phi_1}^{\phi_2} h_\xi h_\phi \, d\xi d\phi. \tag{47}$$

Where $h_\xi$ and $h_\phi$ are the scale factors.

$$A = a^2\sqrt{1-\eta^2}(\phi_2-\phi_1)\int_{\xi_1}^{\xi_2}\sqrt{\xi^2-\eta^2}\,d\xi \tag{48}$$

The integral can be found in Ref. [3, eq. 2.271-3]. The results are

$$A = \frac{a^2}{2}\sqrt{1-\eta^2}(\phi_2-\phi_1)\left[\xi\sqrt{\xi^2-\eta^2} - \eta^2 ln\left(\xi+\sqrt{\xi^2-\eta^2}\right)\right]_{\xi_1}^{\xi_2} \tag{49}$$
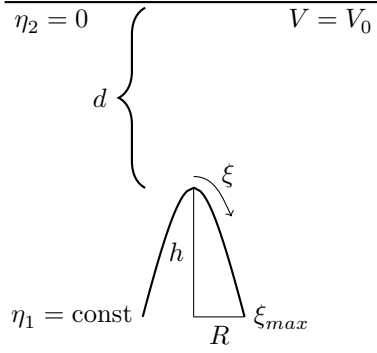
7

Figure 1: Coordinates

### 2.3.3 Arc length

To find the arc length use

$$
\begin{aligned}
x &= a\,sinh\,\mu\,sin\,\nu\,cos\,\phi \\
y &= a\,sinh\,\mu\,sin\,\nu\,sin\,\phi \\
z &= a\,cosh\,\mu\,cos\,\nu
\end{aligned}
\tag{50}
$$

$$
\begin{aligned}
\frac{\partial x}{\partial \mu} &= a\,cosh\,\mu\,sin\,\nu\,cos\,\phi \\
\frac{\partial y}{\partial \mu} &= a\,cosh\,\mu\,sin\,\nu\,sin\,\phi \\
\frac{\partial z}{\partial \mu} &= a\,sinh\,\mu\,cos\,\nu
\end{aligned}
\tag{51}
$$

$$
\begin{aligned}
\left(\frac{\partial x}{\partial \mu}\right)^2 + \left(\frac{\partial y}{\partial \mu}\right)^2 + \left(\frac{\partial z}{\partial \mu}\right)^2 &= a^2\left(cosh^2\,\mu\,sin^2\,\nu + sinh^2\,\mu\,cos^2\,\nu\right) \\
&= sin^2\,\nu + sinh^2\,\mu \\
&= cosh^2\,\mu - cos^2\,\nu
\end{aligned}
\tag{52}
$$

$$
S = \int_0^{\mu_\ell} \sqrt{sin^2\,\nu + sinh^2\,\mu}\;\mathrm{d}\mu
\tag{53}
$$

### 2.3.4 Fixed Tip Size

Define the base radius $R$ and height of the tip $h$ from the base (See Figure 1). We then have

$$
R = a\sqrt{\xi_{max}^2 - 1}\sqrt{1 - \eta_1^2}
\tag{54}
$$

$$
h = -a\xi_{max}\eta - d = -\left(d + a\xi_{max}\eta_1\right)
\tag{55}
$$

and also

$$
\eta_1 = -\frac{d}{a}
\tag{56}
$$

By inserting Equation (56) into Equation (55) we get

$$
\xi_{max} = \frac{h}{d} + 1
\tag{57}
$$

8

We can then use Equation (57) and Equation (54) to obtain

$$a = \sqrt{\frac{d^2 R^2}{h^2 + 2dh} + d^2} \tag{58}$$

It is possible to use Equations (56), (57) and (56) to keep the shape of the tip constant for all $d$.

### 2.3.5 Radius of Curvature

Radius of Curvature is

$$R = \left| \frac{\left( \left( \frac{\mathrm{d}x}{\mathrm{d}\xi} \right)^2 + \left( \frac{\mathrm{d}z}{\mathrm{d}\xi} \right)^2 \right)^{\frac{3}{2}}}{\frac{\mathrm{d}x}{\mathrm{d}\xi} \frac{\mathrm{d}^2 z}{\mathrm{d}\xi^2} - \frac{\mathrm{d}z}{\mathrm{d}\xi} \frac{\mathrm{d}^2 x}{\mathrm{d}\xi^2}} \right| . \tag{59}$$

Set $\phi = 0$ and $\eta = \eta_1$, we then have

$$\frac{\mathrm{d}^2 x}{\mathrm{d}\xi^2} = -a \frac{\sqrt{1 - \eta_1^2}}{(\xi^2 - 1)^{\frac{3}{2}}} \tag{60}$$

and

$$\frac{\mathrm{d}^2 z}{\mathrm{d}\xi^2} = 0 . \tag{61}$$

Therefore,

$$R = \left| \frac{a}{\eta_1} \frac{(\xi^2 - \eta_1^2)^{\frac{3}{2}}}{\sqrt{1 - \eta_1^2}} \right| . \tag{62}$$

If $\xi = 1$ and $\eta_1 = -\frac{a}{d}$ then

$$R = \frac{a^2}{d} - d . \tag{63}$$

### 2.3.6 Normal Vector to Surface

Starting with

$$\xi = \frac{1}{2a} \left( \sqrt{x^2 + y^2 + (z + a)^2} + \sqrt{x^2 + y^2 + (z - a)^2} \right) \tag{64}$$

and inserting this into

$$z = a\xi\eta = \frac{\eta}{2} \left( \sqrt{x^2 + y^2 + (z + a)^2} + \sqrt{x^2 + y^2 + (z - a)^2} \right) . \tag{65}$$

Now solve for $z$ to obtain

$$z = f(x, y) = \frac{\pm \eta}{\sqrt{1 - \eta^2}} \sqrt{x^2 + y^2 + a(1 - \eta^2)} . \tag{66}$$

The normal vector the point $(x_0, y_0)$ is then

$$\vec{N} = [f_x(x_0, y_0), \, f_y(x_0, y_0), \, -1] , \tag{67}$$

or

$$\vec{N} = \left[ \frac{\eta}{\sqrt{1-\eta^2}} \frac{x_0}{\sqrt{x_0^2 + y_0^2 + a^2(1-\eta^2)}}, \; \frac{\eta}{\sqrt{1-\eta^2}} \frac{y_0}{\sqrt{x_0^2 + y_0^2 + a^2(1-\eta^2)}}, \; -1 \right].$$

(68)

This vector points into the surface. Its norm is

$$|\vec{N}|^2 = \frac{1}{1-\eta^2} - \frac{a^2\eta}{x_0^2 + y_0^2 + a^2(1-\eta^2)} \; .$$

(69)

# 3 Cylindrical Geometry

## 3.1 Electric Field

The Laplace equation in cylindrical coordinates is

$$\nabla^2 \Phi = \frac{1}{r}\frac{\delta}{\delta r}\left(r\frac{\delta \Phi}{\delta r}\right) + \frac{1}{r^2}\frac{\delta^2 \Phi}{\delta \theta^2} + \frac{\delta^2 \Phi}{\delta z} = 0 \,. \tag{70}$$

Due to symmetry in $\theta$ and $z$ we have

$$\Phi = \Phi(r) \,, \tag{71}$$

or

$$\nabla^2 \Phi(r) = \frac{1}{r}\frac{\delta}{\delta r}\left(r\frac{\delta \Phi(r)}{\delta r}\right) = 0 \,. \tag{72}$$

Integration yields,

$$\frac{\delta \Phi(r)}{\delta r} = \frac{A}{r} \,, \tag{73}$$

where $A$ is a constant. A second integration then gives,

$$\Phi(r) = A\,ln(r) + B \,, \tag{74}$$

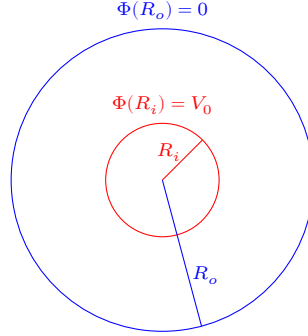where $B$ is also a constant. The boundary conditions seen in Fig. 2 are $\Phi(R_i) = V_0$



Figure 2: A schematic illustration of the system.

and $\Phi(R_o) = 0$. Using them to solve for the constants gives

$$B = V_0 \frac{ln(R_o)}{ln(R_o/R_i)} \,, \tag{75}$$

and

$$A = \frac{V_0}{ln(R_i/R_o)} \,. \tag{76}$$

The electric field is then

$$\vec{E} = -\vec{\nabla}\Phi = -\left(\frac{\delta \Phi}{\delta r}\hat{r} + \frac{1}{r}\frac{\delta \Phi}{\delta \theta}\hat{\theta} + \frac{\delta \Phi}{\delta z}\hat{z}\right) \,, \tag{77}$$

or

$$\vec{E} = \frac{V_0}{ln(R_o/R_i)}\frac{\hat{r}}{r} = \frac{V_0}{ln(R_o/R_i)}\frac{cos(\theta)\hat{x} + sin(\theta)\hat{y}}{r} \,. \tag{78}$$

11

## 3.2  Emission

The emission process checks the angle between the positon vector (black solid line) and the acceleration (violet dashed line) (see Fig. 3). If the angle $\theta$ is greater than $\pi/2$ then emission can occur.
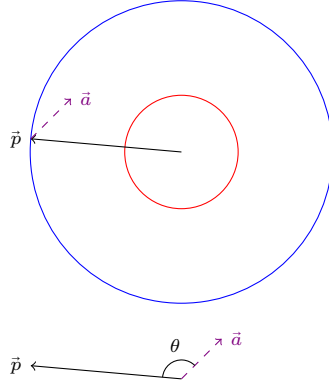
Figure 3: Angle between position and acceleration.

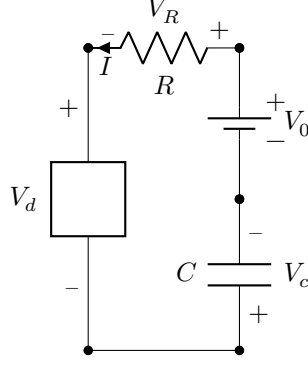# 4 Circuit elements

## 4.1 Series with Resistor and Capacitor



Figure 4: Circuit

For the circuit we have

$$V_0 = V_d + V_R + V_c \tag{79}$$

or

$$V_c(t) = V_0 - V_d - IR. \tag{80}$$

For the capacitor

$$I(t) = C\frac{dV_c(t)}{dt} = C\left[\frac{dV_0(t)}{dt} - \frac{dV_d(t)}{dt} - R\frac{dI(t)}{dt}\right], \tag{81}$$

or

$$-C\frac{dV_d(t)}{dt} = RC\frac{dI(t)}{dt} + I(t), \tag{82}$$

note that $V_0$ is constant in time. Integration from $0$ to $t$ yields,

$$V_d(t) = V_d(0) + R\left[I(0) - I(t)\right] - \frac{1}{C}\int_0^t I(\tau)\,d\tau. \tag{83}$$

The initial conditions $V_d(0) = V_0$ and $I(0) = 0$ give,

$$V_d(t) = V_0 - RI(t) - \frac{1}{C}\int_0^t I(\tau)\,d\tau. \tag{84}$$

The numberical integration can be done using the trapezoidal rule,

$$\int_{t_n}^{t_{n+1}} I(\tau)\,d\tau \approx \Delta t\frac{I(t_n) + I(t_{n+1})}{2}, \tag{85}$$

or

$$\int_0^{t_{n+1}} I(\tau)\,d\tau = \int_0^{t_n} I(\tau)\,d\tau + \int_{t_n}^{t_{n+1}} I(\tau)\,d\tau = \int_0^{t_n} I(\tau)\,d\tau + \Delta t\frac{I(t_n) + I(t_{n+1})}{2}, \tag{86}$$
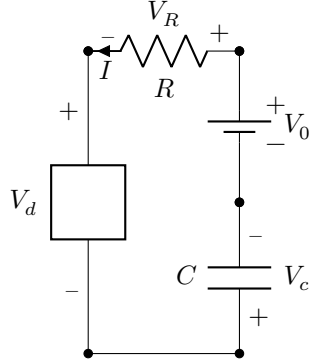
Figure 5: Todo change this figure

## 4.2 Parallel Capacitor

For this circuit we have

$$I = I_d + I_C \,, \tag{87}$$
$$V_d = V_{RC} + V_C \,, \tag{88}$$
$$V_d = V_s - V_R \,, \tag{89}$$
$$I_C = C\frac{dV_C}{dt} \,, \tag{90}$$
$$V_{RC} = R_C I_C \,, \tag{91}$$
$$V_R = RI \,. \tag{92}$$

The goal is to write $V_d$ as a function of $I_d$.

$$V_d = V_s - V_R = V_s - RI = V_s - R(I_d + I_C) = V_s - RI_d - RC\frac{dV_C}{dt} \,. \tag{93}$$

We now get rid of $V_C$ by setting $V_C = V_d - V_{RC}$ to obtain,

$$V_d = V_s - RI_d - RC\frac{dV_d}{dt} + RC\frac{V_{RC}}{dt} \,. \tag{94}$$

Rewriting the equation and using the $V_{RC} = R_C C\frac{dV_C}{dt}$ gives,

$$RC\frac{dV_d}{dt} + V_d = V_s - RI_d + RC\frac{V_{RC}}{dt} = V_s - RI_d + RR_C C^2 \frac{d^2V_C}{dt^2} \,. \tag{95}$$

We again end up with $V_C$ in our equation. To get rid of it we use equation 93,

$$RC\frac{dV_C}{dt} = V_s - RI_d - V_d \,, \tag{96}$$

then taking the derivative and multiplying with $R_C C$,

$$RR_C C^2 \frac{d^2V_C}{dt^2} = -RR_C C\frac{dI_d}{dt} - R_C C\frac{dV_d}{dt} \,. \tag{97}$$

We then obtain,

$$RC\frac{dV_d}{dt} + V_d = V_s - RI_d - RR_C C\frac{dI_d}{dt} - R_C C\frac{dV_d}{dt} \,, \tag{98}$$

or rearranging terms,

$$(R + R_C)C\frac{dV_d}{dt} + V_d = V_s - RI_d - RR_CC\frac{dI_d}{dt} \,. \tag{99}$$

This is a linear differential equation, $\frac{dV_d(t)}{dt} + f(t)V_d(t) = g(t)$, with a general solution given by,

$$V_d(t) = e^{-\int f(t)\,dt}\left(\int g(t)e^{\int f(t)\,dt}\,dt + \kappa\right), \tag{100}$$

where $\kappa$ is a constant determined by the initial conditions $V_d(0) = V_s$, $f(t) = \frac{1}{C(R+R_C)}$ and $g(t) = \frac{1}{C(R+R_C)}\left(V_s + RI_d - RR_CC\frac{dI_d}{dt}\right)$. Let's set $b = C(R + R_C)$, then $\int_0^t f(t')dt' = \frac{t}{b}$. Integration of the terms in $g(t)$ yeilds,

$$\int_0^t V_s e^{t'/b}dt' = bV_s(e^{t/b} - 1), \tag{101}$$

$$\int_0^t \frac{dI_d}{dt'}e^{t'/b}dt' = \left[e^{t'/b}I_d\right]_0^t - \frac{1}{b}\int_0^t I_d e^{t'/b}dt' = I_d e^{t/b}I_d(0) - \frac{1}{b}\int_0^t I_d e^{t'/b}dt' \,. \tag{102}$$

The solutions the becomes,

$$V_d(t) = \frac{1}{b}e^{-t/b}\left[bV_s\left(e^{t/b} - 1\right) - R\int_0^t I_d e^{t'/b}dt' - RR_CC\left(I_d e^{t/b} - I_d(0) - \frac{1}{b}\int_0^t I_d e^{t'/b}dt'\right) + \kappa\right], \tag{103}$$

or

$$V_d(t) = \frac{1}{b}e^{-t/b}\left[bV_s\left(e^{t/b} - 1\right) - \left(R - \frac{RR_CC}{b}\right)\int_0^t I_d e^{t'/b}dt' - RR_CC\left(I_d e^{t/b} - I_d(0)\right) + \kappa\right]. \tag{104}$$

Using the initial conditions $V_d(0) = V_s$ and $I_d(0) = 0$ gives $\kappa = bV_s$,

$$V_d(t) = e^{-t/b}\left[V_s e^{t/b} - \frac{1}{b}\left(R - \frac{RR_CC}{b}\right)\int_0^t I_d e^{t'/b}dt' - \frac{RR_CC}{b}I_d e^{t/b}\right]. \tag{105}$$

In the end we get

$$V_d(t) = V_s - \frac{R^2}{(R + R_C)^2 C}\int_0^t I_d(t')e^{\frac{t'-t}{C(R+R_C)}}dt' - \frac{RR_C}{R + R_C}I_d(t). \tag{106}$$

For the numerical integration we have

$$\int_{t_n}^{t_{n+1}} I(t')e^{\frac{t'-t_{n+1}}{C(R+R_C)}}dt' = \frac{\Delta t}{2}\left(I(t_n)e^{-\frac{\Delta t}{C(R+R_C)}} + I(t_{n+1})\right). \tag{107}$$

# References

[1] Richard G Forbes and Jonathan H.B Deane. "Reformulation of the standard theory of Fowler–Nordheim tunnelling and cold field electron emission". In: *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Science* 463.2087 (2007), pp. 2907–2927. DOI: 10.1098/rspa.2007.0030. eprint: http://rspa.royalsocietypublishing.org/content/463/2087/2907.full.pdf+html. URL: http://rspa.royalsocietypublishing.org/content/463/2087/2907.abstract.

[2] Li-Hong Pan et al. "Three-dimensional electrostatic potential, and potential-energy barrier, near a tip-base junction". In: *Applied Physics Letters* 65.17 (1994), pp. 2151–2153. DOI: 10.1063/1.112775. URL: http://link.aip.org/link/?APL/65/2151/1.

[3] IS Gradshtein IM Ryshik, IS Gradstein, and A Jeffrey. *Table of Integrals, Series and Products*. 2007.

[4] Q Spreiter and M Walter. "Classical Molecular Dynamics Simulation with the Velocity Verlet Algorithm at Strong External Magnetic Fields". In: *Journal of Computational Physics* 152.1 (1999), pp. 102–119. ISSN: 0021-9991. DOI: 10.1006/jcph.1999.6237. URL: http://www.sciencedirect.com/science/article/pii/S002199919996237X.