Notes on Vacuum Electronics Molecular Dynamics Simulations

Kristinn Torfason

September 4, 2017

1 Verlet Integration

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

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

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

Force on a particle due to an electric field

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

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,

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

then calculate the acceleration a_{n+1} using x_{n+1} and finally 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,

$$\bar{x}_{n+1} = \bar{x}_n + \bar{v}_n \Delta \bar{t} + \frac{1}{2} \bar{a}_n \Delta \bar{t}^2$$
, (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 $L=1.0*10^{-9}\,\mathrm{m}$ and $T=1.0*10^{-12}\,\mathrm{s}$, 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

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

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

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

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,

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

1.2 Unit Test Case

Two electrons and one hole.

Fyrst electron: $x_1=10\,\mathrm{nm},\,y_1=3\,\mathrm{nm},\,z_1=100\,\mathrm{nm}.$

Second electron: $x_2=35\,\mathrm{nm},\,y_2=-7\,\mathrm{nm},\,z_2=10\,\mathrm{nm}.$

The hole: $x_3=-12\,\mathrm{nm},\,y_3=0\,\mathrm{nm},\,z_3=50\,\mathrm{nm}.$

Parameters: d100 nm, V=2 V, $\Delta t=0.25$ ps.

The acceleration of the fyrst electron is

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

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

2 Field Emission

2.1 Fowler-Nordheim equation

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

where $a \approx 1.541434 \times 10^{-6} \text{ AeVV}^{-2}$ and $b \approx 6.830890 \text{ eV}^{-3/2} \text{Vnm}^{-1}$ 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 ϕ 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 ${\rm AJV^{-2}}$. If we convert to ${\rm AeVV^{-2}}$ 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 $\rm J^{-3/2}Vm^{-1}$. If we convert it to $\rm eV^{-3/2}Vm^{-1}$ then we must multiply it with a factor of $(1/e)^{-3/2}$ and obtain

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

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

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

Calculated iteratively

2.3 Prolate spheroidal coordinates

The prolate spheroidal coordinates are defined as

$$x = a \sinh \mu \sin \nu \cos \phi$$

$$y = a \sinh \mu \sin \nu \sin \phi$$

$$z = a \cosh \mu \cos \nu$$
(28)

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

$$sinh^{2} \mu = cosh^{2} \mu - 1 = \xi^{2} - 1
sin^{2} \nu = 1 - cos^{2} \nu = 1 - \eta^{2}$$
(29)

which gives

$$x = a\sqrt{\xi^2 - 1}\sqrt{1 - \eta^2}\cos\phi$$

$$y = a\sqrt{\xi^2 - 1}\sqrt{1 - \eta^2}\sin\phi$$

$$z = a\xi\eta$$
(30)

The reverse are

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

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

$$\phi = \arctan \frac{y}{x}$$
(31)

To find ξ or z if given x and y

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

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

Derivatives of the coordinates

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

The gradient is

$$\nabla V(\xi, \eta, \phi) = \hat{x} \frac{\partial V}{\partial x} + \hat{y} \frac{\partial V}{\partial y} + \hat{z} \frac{\partial V}{\partial z}$$

$$= \hat{x} \left(\frac{\partial V}{\partial \xi} \frac{\partial \xi}{x} + \frac{\partial V}{\partial \eta} \frac{\partial \eta}{x} + \frac{\partial V}{\partial \phi} \frac{\partial \phi}{x} \right)$$

$$+ \hat{y} \left(\frac{\partial V}{\partial \xi} \frac{\partial \xi}{y} + \frac{\partial V}{\partial \eta} \frac{\partial \eta}{y} + \frac{\partial V}{\partial \phi} \frac{\partial \phi}{y} \right)$$

$$+ \hat{z} \left(\frac{\partial V}{\partial \xi} \frac{\partial \xi}{z} + \frac{\partial V}{\partial \eta} \frac{\partial \eta}{z} + \frac{\partial V}{\partial \phi} \frac{\partial \phi}{z} \right)$$
(35)

The position vector is

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

and the unit vector are then

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

For $\hat{\eta}$ we have

$$\hat{\eta} = \sqrt{\frac{1 - \eta^2}{\xi^2 - \eta^2}} \begin{pmatrix} -\eta \sqrt{\frac{\xi^2 - 1}{1 - \eta^2}} \cos \phi \\ -\eta \sqrt{\frac{\xi^2 - 1}{1 - \eta^2}} \sin \phi \\ \xi \end{pmatrix}$$
(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 η_1

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

2.3.1 Electric Field for Hyperbolid Tip

The vector potential is [2]

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

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

The gradient in Prolate-Spherodial coordinates is

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

and the electric field is

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

Here ξ , η and ϕ are the position inside the diode. While η_1 is the hyberbolid tip and $\eta_2 = 0$ is the anode plane.

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

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

Where h_{ξ} and h_{ϕ} are the scale factors.

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

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

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

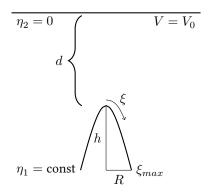


Figure 1: Coordinates

2.3.3 Arc length

To find the arc length use

$$x = a \sinh \mu \sin \nu \cos \phi$$

$$y = a \sinh \mu \sin \nu \sin \phi$$

$$z = a \cosh \mu \cos \nu$$
(50)

$$\frac{\partial x}{\partial \mu} = a \cosh \mu \sin \nu \cos \phi$$

$$\frac{\partial y}{\partial \mu} = a \cosh \mu \sin \nu \sin \phi$$

$$\frac{\partial z}{\partial \mu} = a \sinh \mu \cos \nu$$
(51)

$$\left(\frac{\partial x}{\partial \mu}\right)^{2} + \left(\frac{\partial y}{\partial \mu}\right)^{2} + \left(\frac{\partial z}{\partial \mu}\right)^{2} = a^{2} \left(\cosh^{2} \mu \sin^{2} \nu + \sinh^{2} \mu \cos^{2} \nu\right)$$

$$= \sin^{2} \nu + \sinh^{2} \mu$$

$$= \cosh^{2} \mu - \cos^{2} \nu$$
(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

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

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

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

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

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

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

The normal vector the point $\left(x_{0},y_{0}\right)$ is then

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

or

$$\vec{N} = \left[\frac{\eta}{\sqrt{1-\eta^2}} \frac{x_0}{\sqrt{x_0^2 + y_0^2 + a^2(1-\eta^2)}}, \, \frac{\eta}{\sqrt{1-\eta^2}} \frac{y_0}{\sqrt{x_0^2 + y_0^2 + a^2(1-\eta^2)}}, \, -1 \right] \, . \tag{(3)}$$

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

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

Due to symmetry in θ 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 $\Phi(R_i) = V_0$

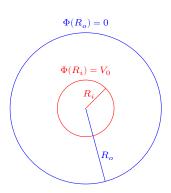


Figure 2: A schematic illustration of the system.

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

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

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

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

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 θ is greater than $\pi/2$ then emission can occur.

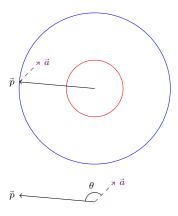


Figure 3: Angle between position and acceleration.

4 Circuit elements

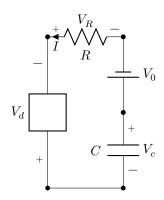


Figure 4: Circuit

For the circut we have

$$V_d(t) = V + V_c(t), (79)$$

or

$$V_c(t) = V_d(t) - V$$
 . (80)

For the capacitor

$$I(t) = C \frac{dV_c(t)}{dt} = C \frac{dV_d(t)}{dt} \,, \tag{81} \label{eq:81}$$

because V is constant. Integration from 0 to t then gives

$$V_{d}(t) = V_{d}(0) + C \int_{0}^{t} I(t')dt' , \qquad (82)$$

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.