

Notes on Vacuum Electronics Molecular Dynamics Simulations

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1 Verlet Integration

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

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

$$\mathbf{F}(\mathbf{r}) = \frac{q^2}{4\pi\epsilon_0} \sum_{i=1}^N \frac{\mathbf{r} - \mathbf{r}_i}{|\mathbf{r} - \mathbf{r}_i|^3} \quad (2)$$

Force on a particle due to an electric field

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

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

$$F_z = qE_z = q\frac{V}{d}, \quad (4)$$

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

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

where v_0 is the initial velocity.

1.1 Velocity Verlet

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

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

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

$$v_{n+1} = v_n + \frac{a_n + a_{n+1}}{2} \Delta t. \quad (7)$$

Note this method assumes that a_{n+1} does 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 weak, see also [4].

1.1.1 Nondimensionalization

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

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

and,

$$\bar{v}_{n+1} = \bar{v}_n + \frac{\bar{a}_n + \bar{a}_{n+1}}{2} \bar{\Delta t}. \quad (9)$$

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,

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

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

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

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

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

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

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

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,

$$\bar{a} = \frac{qV}{m\bar{d}} \frac{T^2}{L^2}. \quad (14)$$

2 Field Emission

2.1 Fowler-Nordheim equation

$$J = \frac{a}{\phi t^2(l)} F^2 \exp(-\nu(l)b\phi^{3/2}/F) \quad (15)$$

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 (20) and (21)).

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

$$\nu(l) = 1 - l + \frac{1}{6} l \ln(l) \quad (16)$$

and for $t(l)$

$$t(l) = 1 + l \left(\frac{1}{9} - \frac{1}{18} \ln(l) \right) \quad (17)$$

where

$$l = \frac{F}{F_\phi} = \frac{e^3}{4\pi\epsilon_0} \frac{F}{\phi^2} \quad (18)$$

If ϕ is in eV and F in V/m then

$$l = \frac{e}{4\pi\epsilon_0} \frac{F}{\phi^2} \quad (19)$$

The first Fowler-Nordheim constant is in SI units

$$a_{FN} = \frac{e^3}{8\pi h} \quad (20)$$

and has units $\text{A}\cdot\text{J}\cdot\text{V}^{-2}$. If we convert to $\text{AeV}\cdot\text{V}^{-2}$ then we must multiply with $1/e$ to obtain

$$a_{FN} = \frac{e^2}{8\pi\hbar} = \frac{e^2}{16\pi^2\hbar} \quad (21)$$

The second Fowler-Nordheim constant is in SI units

$$b_{FN} = \frac{8\pi}{3e\hbar} \sqrt{2m_e} \quad (22)$$

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

$$b_{FN} = \frac{8\pi\sqrt{2m_e}e}{3\hbar} = \frac{4}{3\hbar} \sqrt{2em_e} \quad (23)$$

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

$$E = E_0 + 2 \int_0^d \int_{-\frac{L}{2}}^{\frac{L}{2}} \int_{-\frac{L}{2}}^{\frac{L}{2}} \frac{1}{4\pi\epsilon_0} \frac{z\sigma(z)}{(x^2 + y^2 + z^2)^{3/2}} dx dy dz. \quad (24)$$

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

$$E = 1 - \frac{2J}{9\pi} \int_0^1 \int_{-\frac{L}{2d}}^{\frac{L}{2d}} \int_{-\frac{L}{2d}}^{\frac{L}{2d}} \frac{\sqrt{\hat{z}}}{(\hat{x}^2 + \hat{y}^2 + \hat{z}^2)^{3/2}} d\hat{x} d\hat{y} d\hat{z}. \quad (25)$$

Calculated iteratively

2.3 Prolate spheroidal coordinates

The prolate spheroidal coordinates are defined as

$$\begin{aligned}x &= a \sinh \mu \sin \nu \cos \phi \\y &= a \sinh \mu \sin \nu \sin \phi \\z &= a \cosh \mu \cos \nu\end{aligned}\tag{26}$$

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

$$\begin{aligned}\sinh^2 \mu &= \cosh^2 \mu - 1 = \xi^2 - 1 \\ \sin^2 \nu &= 1 - \cos^2 \nu = 1 - \eta^2\end{aligned}\tag{27}$$

which gives

$$\begin{aligned}x &= a \sqrt{\xi^2 - 1} \sqrt{1 - \eta^2} \cos \phi \\y &= a \sqrt{\xi^2 - 1} \sqrt{1 - \eta^2} \sin \phi \\z &= a \xi \eta\end{aligned}\tag{28}$$

The reverse are

$$\begin{aligned}\xi &= \frac{1}{2a} \left(\sqrt{x^2 + y^2 + (z+a)^2} + \sqrt{x^2 + y^2 + (z-a)^2} \right) \\ \eta &= \frac{1}{2a} \left(\sqrt{x^2 + y^2 + (z+a)^2} - \sqrt{x^2 + y^2 + (z-a)^2} \right) \\ \phi &= \arctan \frac{y}{x}\end{aligned}\tag{29}$$

To find ξ or z if given x and y

$$\xi = \frac{1}{a \sqrt{1 - \eta^2}} \sqrt{x^2 + y^2 + a^2(1 - \eta^2)}\tag{30}$$

$$z = \frac{\eta}{\sqrt{1 - \eta^2}} \sqrt{x^2 + y^2 + a^2(1 - \eta^2)}\tag{31}$$

Derivatives of the coordinates

$$\begin{aligned}\frac{\partial x}{\partial \xi} &= a \xi \frac{\sqrt{1 - \eta^2}}{\sqrt{\xi^2 - 1}} \cos \phi, & \frac{\partial y}{\partial \xi} &= a \xi \frac{\sqrt{1 - \eta^2}}{\sqrt{\xi^2 - 1}} \sin \phi, & \frac{\partial z}{\partial \xi} &= a \eta, \\ \frac{\partial x}{\partial \eta} &= -a \eta \frac{\sqrt{\xi^2 - 1}}{\sqrt{1 - \eta^2}} \cos \phi, & \frac{\partial y}{\partial \eta} &= -a \eta \frac{\sqrt{\xi^2 - 1}}{\sqrt{1 - \eta^2}} \sin \phi, & \frac{\partial z}{\partial \eta} &= a \xi, \\ \frac{\partial x}{\partial \phi} &= -a \sqrt{\xi^2 - 1} \sqrt{1 - \eta^2} \sin \phi, & \frac{\partial y}{\partial \phi} &= a \sqrt{\xi^2 - 1} \sqrt{1 - \eta^2} \cos \phi, & \frac{\partial z}{\partial \phi} &= 0.\end{aligned}\tag{32}$$

The gradient is

$$\begin{aligned}\nabla V(\xi, \eta, \phi) &= \hat{x} \frac{\partial V}{\partial x} + \hat{y} \frac{\partial V}{\partial y} + \hat{z} \frac{\partial V}{\partial z} \\ &= \hat{x} \left(\frac{\partial V}{\partial \xi} \frac{\partial \xi}{\partial x} + \frac{\partial V}{\partial \eta} \frac{\partial \eta}{\partial x} + \frac{\partial V}{\partial \phi} \frac{\partial \phi}{\partial x} \right) \\ &+ \hat{y} \left(\frac{\partial V}{\partial \xi} \frac{\partial \xi}{\partial y} + \frac{\partial V}{\partial \eta} \frac{\partial \eta}{\partial y} + \frac{\partial V}{\partial \phi} \frac{\partial \phi}{\partial y} \right) \\ &+ \hat{z} \left(\frac{\partial V}{\partial \xi} \frac{\partial \xi}{\partial z} + \frac{\partial V}{\partial \eta} \frac{\partial \eta}{\partial z} + \frac{\partial V}{\partial \phi} \frac{\partial \phi}{\partial z} \right)\end{aligned}\tag{33}$$

The position vector is

$$\vec{r} = \begin{pmatrix} a\sqrt{(\xi^2-1)(1-\eta^2)} \cos \phi \\ a\sqrt{(\xi^2-1)(1-\eta^2)} \sin \phi \\ a\xi\eta \end{pmatrix}, \quad (34)$$

and the unit vector are then

$$\hat{\xi} = \frac{\frac{d\vec{r}}{d\xi}}{\left|\frac{d\vec{r}}{d\xi}\right|}, \quad \hat{\eta} = \frac{\frac{d\vec{r}}{d\eta}}{\left|\frac{d\vec{r}}{d\eta}\right|}, \quad \hat{\phi} = \frac{\frac{d\vec{r}}{d\phi}}{\left|\frac{d\vec{r}}{d\phi}\right|}. \quad (35)$$

For $\hat{\eta}$ we have

$$\hat{\eta} = \sqrt{\frac{1-\eta^2}{\xi^2-\eta^2}} \begin{pmatrix} -\eta\sqrt{\frac{\xi^2-1}{1-\eta^2}} \cos \phi \\ -\eta\sqrt{\frac{\xi^2-1}{1-\eta^2}} \sin \phi \\ \xi \end{pmatrix} \quad (36)$$

Scale factors are

$$h_\xi = a\sqrt{\frac{\xi^2-\eta^2}{\xi^2-1}}, \quad h_\eta = a\sqrt{\frac{\xi^2-\eta^2}{1-\eta^2}}, \quad h_\phi = a\sqrt{(\xi^2-1)(1-\eta^2)} \quad (37)$$

Given x, y and η_1

$$\xi = \frac{1}{a} \frac{1}{\sqrt{1-\eta_1^2}} \sqrt{x^2 + y^2 + a^2(1-\eta_1^2)} \quad (38)$$

2.4 Electric field for hyperboloid tip

The vector potential is [2]

$$V(\eta) = V_0 \frac{\ln \left[\frac{1+\eta_1}{1-\eta_1} \frac{1-\eta}{1+\eta} \right]}{\ln \left[\frac{1+\eta_1}{1-\eta_1} \frac{1-\eta_2}{1+\eta_2} \right]}. \quad (39)$$

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

$$\frac{dV(\eta)}{d\eta} = -\frac{2V_0}{1-\eta^2} \ln^{-1} \left[\frac{1+\eta_1}{1-\eta_1} \frac{1-\eta_2}{1+\eta_2} \right] \quad (40)$$

The gradient in Prolate-Spheroidal coordinates is

$$\nabla V(\eta) = \frac{1}{a} \sqrt{\frac{1-\eta^2}{\xi^2-\eta^2}} \frac{dV(\eta)}{d\eta} \hat{\eta}, \quad (41)$$

and the electric field is

$$\vec{E} = -\nabla V(\eta) = \frac{2V_0}{a} \frac{1}{\xi^2-\eta^2} \frac{1}{\ln \left[\frac{1+\eta_1}{1-\eta_1} \frac{1-\eta_2}{1+\eta_2} \right]} \begin{pmatrix} -\eta\sqrt{\frac{\xi^2-1}{1-\eta^2}} \cos \phi \\ -\eta\sqrt{\frac{\xi^2-1}{1-\eta^2}} \sin \phi \\ \xi \end{pmatrix} \quad (42)$$

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

$$|\vec{E}| = \frac{2V_0}{a} \frac{1}{\sqrt{\xi^2 - \eta^2} \sqrt{1 - \eta^2}} \frac{1}{\ln \left[\frac{1+\eta_1}{1-\eta_1} \frac{1-\eta_2}{1+\eta_2} \right]} \quad (43)$$

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

$$E_z = \frac{2V_0}{a} \frac{1}{1 - \eta_1^2} \frac{1}{\ln \left[\frac{1+\eta_1}{1-\eta_1} \right]}. \quad (44)$$

2.5 Area calculations for hyperboloid tip

The Surface area is given by the integral

$$A = \int_{\xi_1}^{\xi_2} \int_{\phi_1}^{\phi_2} h_\xi h_\phi d\xi d\phi. \quad (45)$$

Where h_ξ and h_ϕ are the scale factors.

$$A = a^2 \sqrt{1 - \eta^2} (\phi_2 - \phi_1) \int_{\xi_1}^{\xi_2} \sqrt{\xi^2 - \eta^2} d\xi \quad (46)$$

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

$$A = \frac{a^2}{2} \sqrt{1 - \eta^2} (\phi_2 - \phi_1) \left[\xi \sqrt{\xi^2 - \eta^2} - \eta^2 \ln \left(\xi + \sqrt{\xi^2 - \eta^2} \right) \right]_{\xi_1}^{\xi_2} \quad (47)$$

2.6 Arc length

To find the arc length use

$$\begin{aligned} x &= a \sinh \mu \sin \nu \cos \phi \\ y &= a \sinh \mu \sin \nu \sin \phi \\ z &= a \cosh \mu \cos \nu \end{aligned} \quad (48)$$

$$\begin{aligned} \frac{\partial x}{\partial \mu} &= a \cosh \mu \sin \nu \cos \phi \\ \frac{\partial y}{\partial \mu} &= a \cosh \mu \sin \nu \sin \phi \\ \frac{\partial z}{\partial \mu} &= a \sinh \mu \cos \nu \end{aligned} \quad (49)$$

$$\begin{aligned} \left(\frac{\partial x}{\partial \mu} \right)^2 + \left(\frac{\partial y}{\partial \mu} \right)^2 + \left(\frac{\partial z}{\partial \mu} \right)^2 &= a^2 (\cosh^2 \mu \sin^2 \nu + \sinh^2 \mu \cos^2 \nu) \\ &= \sin^2 \nu + \sinh^2 \mu \\ &= \cosh^2 \mu - \cos^2 \nu \end{aligned} \quad (50)$$

$$S = \int_0^{\mu_\ell} \sqrt{\sin^2 \nu + \sinh^2 \mu} d\mu \quad (51)$$

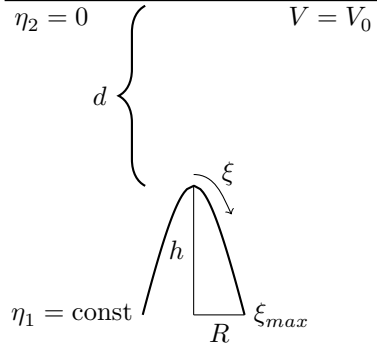


Figure 1: Coordinates

2.7 Fixed tip size

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

$$R = a\sqrt{\xi_{max}^2 - 1}\sqrt{1 - \eta_1^2} \quad (52)$$

$$h = -a\xi_{max}\eta - d = -(d + a\xi_{max}\eta_1) \quad (53)$$

and also

$$\eta_1 = -\frac{d}{a} \quad (54)$$

By inserting Equation (54) into Equation (53) we get

$$\xi_{max} = \frac{h}{d} + 1 \quad (55)$$

We can then use Equation (55) and Equation (52) to obtain

$$a = \sqrt{\frac{d^2 R^2}{h^2 + 2dh} + d^2} \quad (56)$$

It is possible to use Equations (54), (55) and (54) to keep the shape of the tip constant for all d .

2.8 Radius of Curvature

Radius of Curvature is

$$R = \left| \frac{\left(\left(\frac{dx}{d\xi} \right)^2 + \left(\frac{dz}{d\xi} \right)^2 \right)^{\frac{3}{2}}}{\frac{dx}{d\xi} \frac{d^2 z}{d\xi^2} - \frac{dz}{d\xi} \frac{d^2 x}{d\xi^2}} \right|. \quad (57)$$

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

$$\frac{d^2 x}{d\xi^2} = -a \frac{\sqrt{1 - \eta_1^2}}{(\xi^2 - 1)^{\frac{3}{2}}} \quad (58)$$

and

$$\frac{d^2 z}{d\xi^2} = 0. \quad (59)$$

Therefore,

$$R = \left| \frac{a}{\eta_1} \frac{(\xi^2 - \eta_1^2)^{\frac{3}{2}}}{\sqrt{1 - \eta_1^2}} \right|. \quad (60)$$

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

$$R = \frac{a^2}{d} - d. \quad (61)$$

2.9 Normal Vector to surface

Starting with

$$\xi = \frac{1}{2a} \left(\sqrt{x^2 + y^2 + (z+a)^2} + \sqrt{x^2 + y^2 + (z-a)^2} \right) \quad (62)$$

and inserting this into

$$z = a\xi\eta = \frac{\eta}{2} \left(\sqrt{x^2 + y^2 + (z+a)^2} + \sqrt{x^2 + y^2 + (z-a)^2} \right). \quad (63)$$

Now solve for z to obtain

$$z = f(x, y) = \frac{\pm\eta}{\sqrt{1-\eta^2}} \sqrt{x^2 + y^2 + a(1-\eta^2)}. \quad (64)$$

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

$$\vec{N} = [f_x(x_0, y_0), f_y(x_0, y_0), -1], \quad (65)$$

or

$$\vec{N} = \left[\frac{\eta}{\sqrt{1-\eta^2}} \frac{x_0}{\sqrt{x_0^2 + y_0^2 + a^2(1-\eta^2)}}, \frac{\eta}{\sqrt{1-\eta^2}} \frac{y_0}{\sqrt{x_0^2 + y_0^2 + a^2(1-\eta^2)}}, -1 \right]. \quad (66)$$

This vector points into the surface. Its norm is

$$|\vec{N}|^2 = \frac{1}{1-\eta^2} - \frac{a^2\eta}{x_0^2 + y_0^2 + a^2(1-\eta^2)}. \quad (67)$$

2.10 Circuit elements

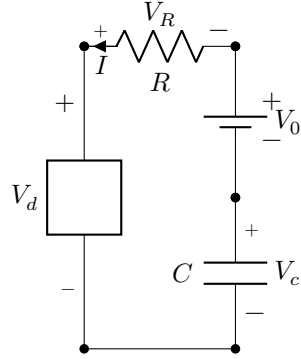


Figure 2: Circuit

For the circuit we have

$$V_d(t) = V + V_c(t), \quad (68)$$

or

$$V_c(t) = V_d(t) - V. \quad (69)$$

For the capacitor

$$I(t) = C \frac{dV_c(t)}{dt} = C \frac{dV_d(t)}{dt}, \quad (70)$$

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

$$V_d(t) = V_d(0) + C \int_0^t I(t') dt', \quad (71)$$

3 Cylindrical Geometry

3.1 Electric Field

The Laplace equation in cylindrical coordinates is

$$\nabla^2 \Phi = \frac{1}{r} \frac{\delta}{\delta r} \left(r \frac{\delta \Phi}{\delta r} \right) + \frac{1}{r^2} \frac{\delta^2 \Phi}{\delta \theta^2} + \frac{\delta^2 \Phi}{\delta z^2} = 0. \quad (72)$$

Due to symmetry in θ and z we have

$$\Phi = \Phi(r), \quad (73)$$

or

$$\nabla^2 \Phi(r) = \frac{1}{r} \frac{\delta}{\delta r} \left(r \frac{\delta \Phi(r)}{\delta r} \right) = 0. \quad (74)$$

Integration yields,

$$\frac{\delta \Phi(r)}{\delta r} = \frac{A}{r}, \quad (75)$$

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

$$\Phi(r) = A \ln(r) + B, \quad (76)$$

where B is also a constant. The boundary conditions seen in Fig. 3 are $\Phi(R_i) = V_0$

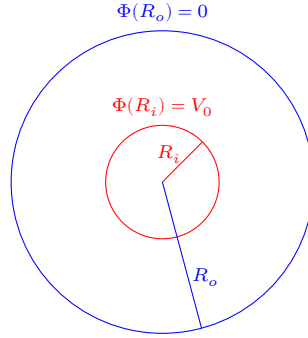


Figure 3: A schematic illustration of the system.

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

$$B = V_0 \frac{\ln(R_o)}{\ln(R_o/R_i)}, \quad (77)$$

and

$$A = \frac{V_0}{\ln(R_i/R_o)}. \quad (78)$$

The electric field is then

$$\vec{E} = -\vec{\nabla} \Phi = - \left(\frac{\delta \Phi}{\delta r} \hat{r} + \frac{1}{r} \frac{\delta \Phi}{\delta \theta} \hat{\theta} + \frac{\delta \Phi}{\delta z} \hat{z} \right), \quad (79)$$

or

$$\vec{E} = \frac{V_0}{\ln(R_o/R_i)} \frac{\hat{r}}{r} = \frac{V_0}{\ln(R_o/R_i)} \frac{\cos(\theta)\hat{x} + \sin(\theta)\hat{y}}{r}. \quad (80)$$

3.2 Emission

The emission process checks the angle between the position vector (black solid line) and the acceleration (violet dashed line) (see Fig. 4). If the angle θ is greater than $\pi/2$ then emission can occur.

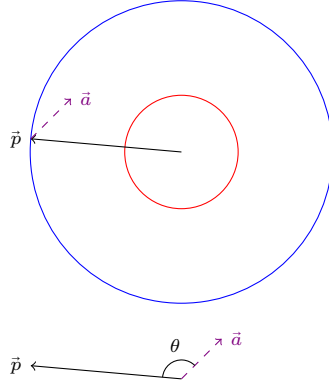


Figure 4: Angle between position and acceleration.

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