Image-Force Barrier Lowering of Contact Resistance for Two-Dimensional Materials:
Direct Determination and Method of Images on a Cone Manifold

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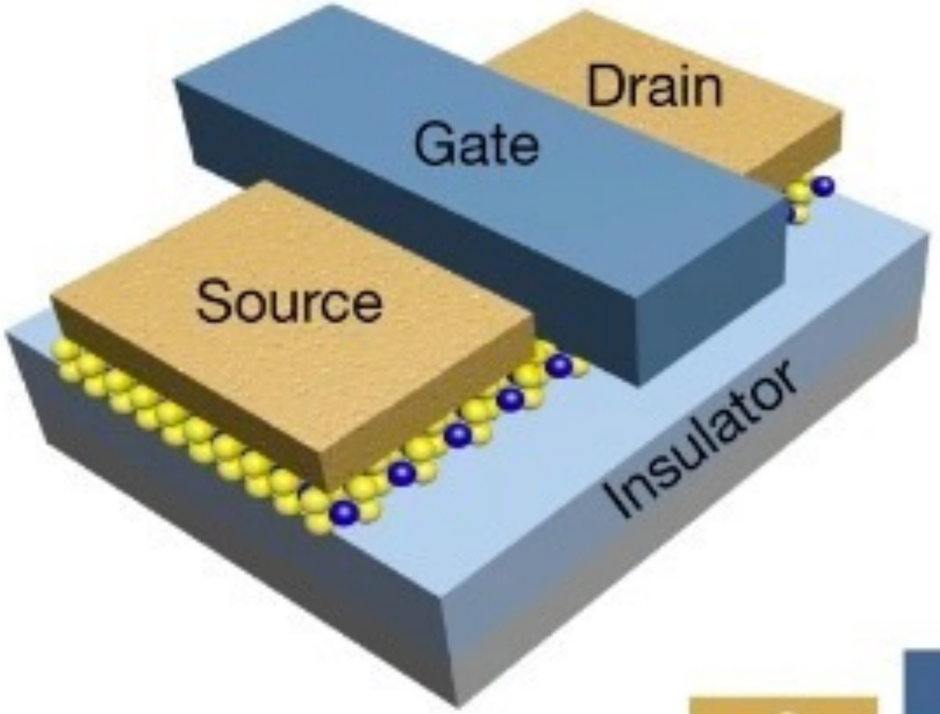
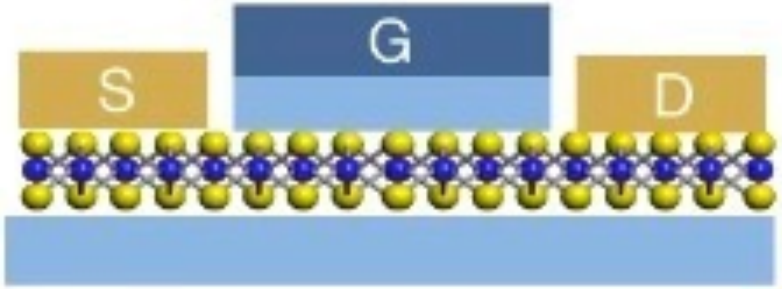
1 2 3 4

Introduction

- 2D Materials
  - TMD as channel material

- Limited by high:
  - Schottky barriers
  - Contact Resistance (R_C)

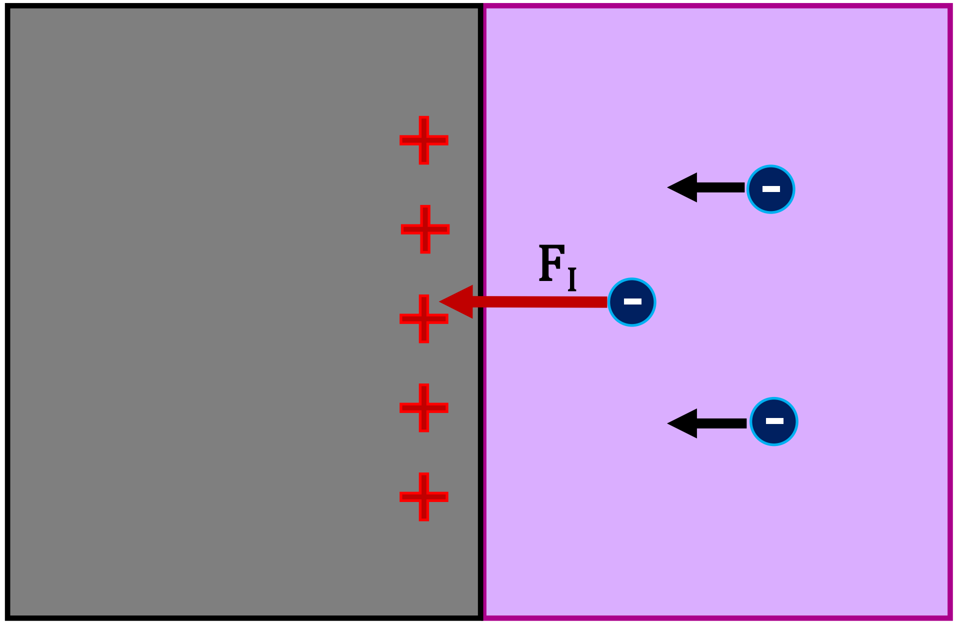


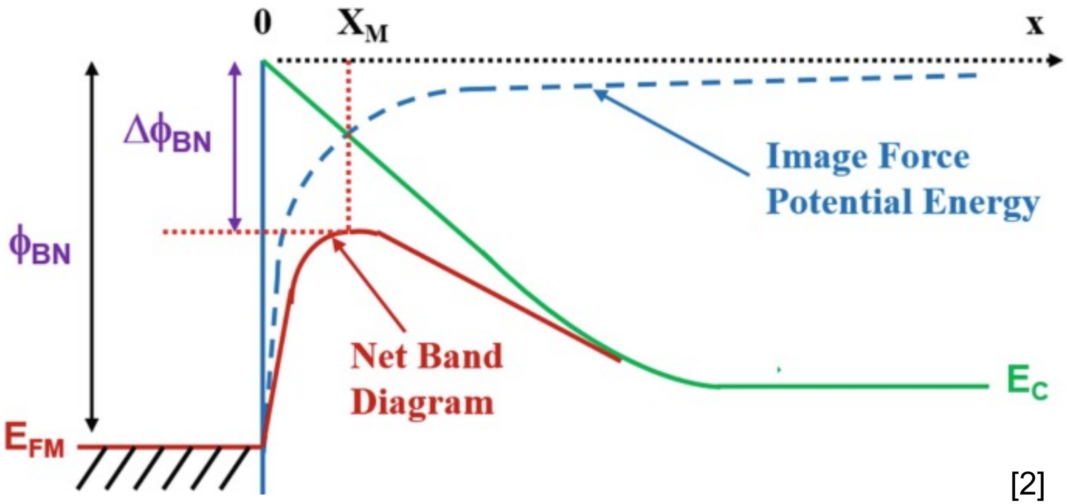


2D FET (ultimate body scaling)

[1] Y. Liu, *et al.*, "Promises and prospects of two-dimensional transistors," Nature, 2021

Image Force Barrier Lowering (IFBL)

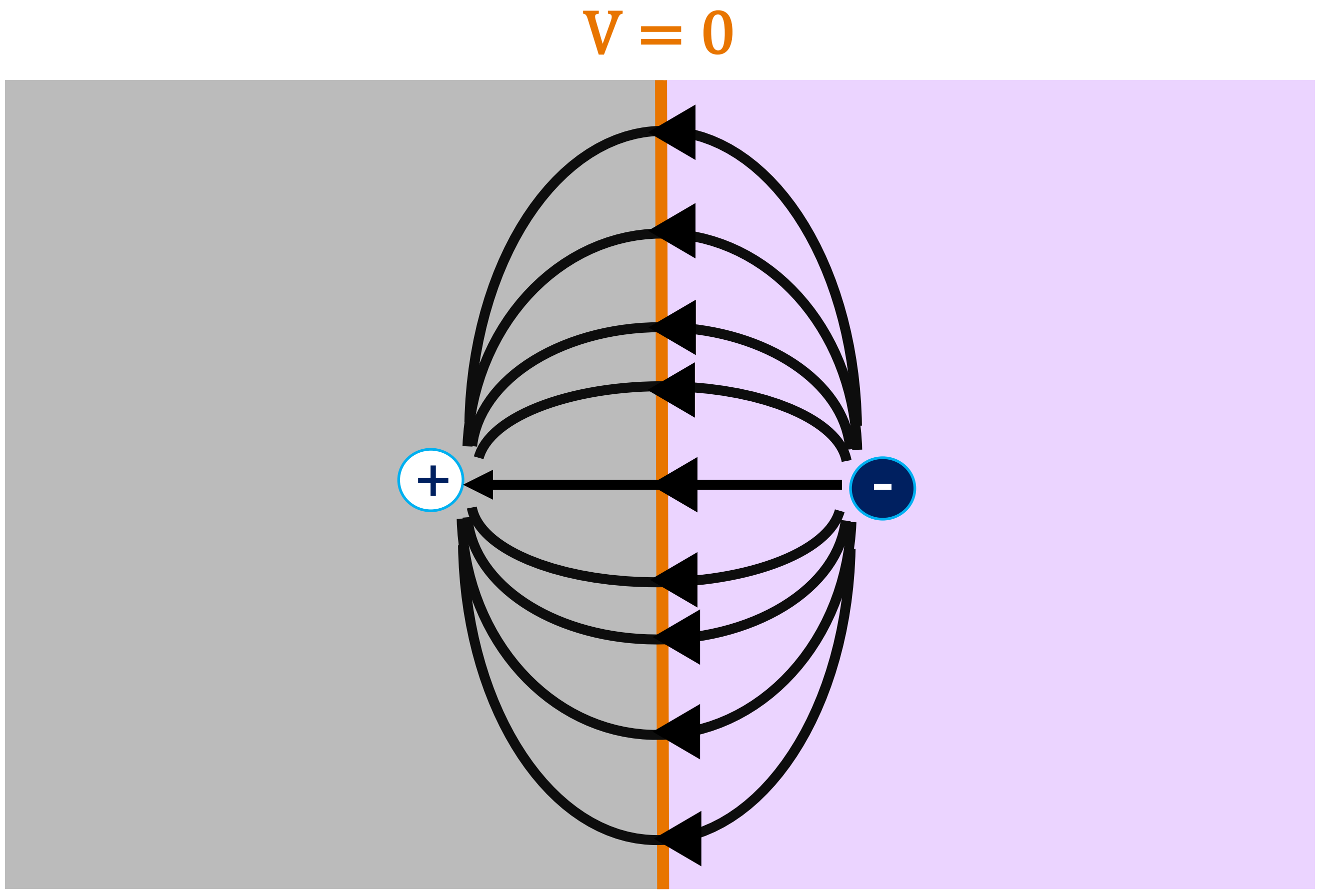




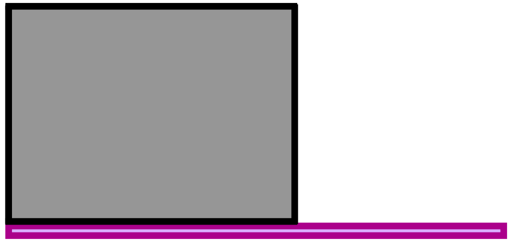
[2] Baliga, B.J., *Springer* (2019).

How can we solve for IFBL?

- Method of Images!



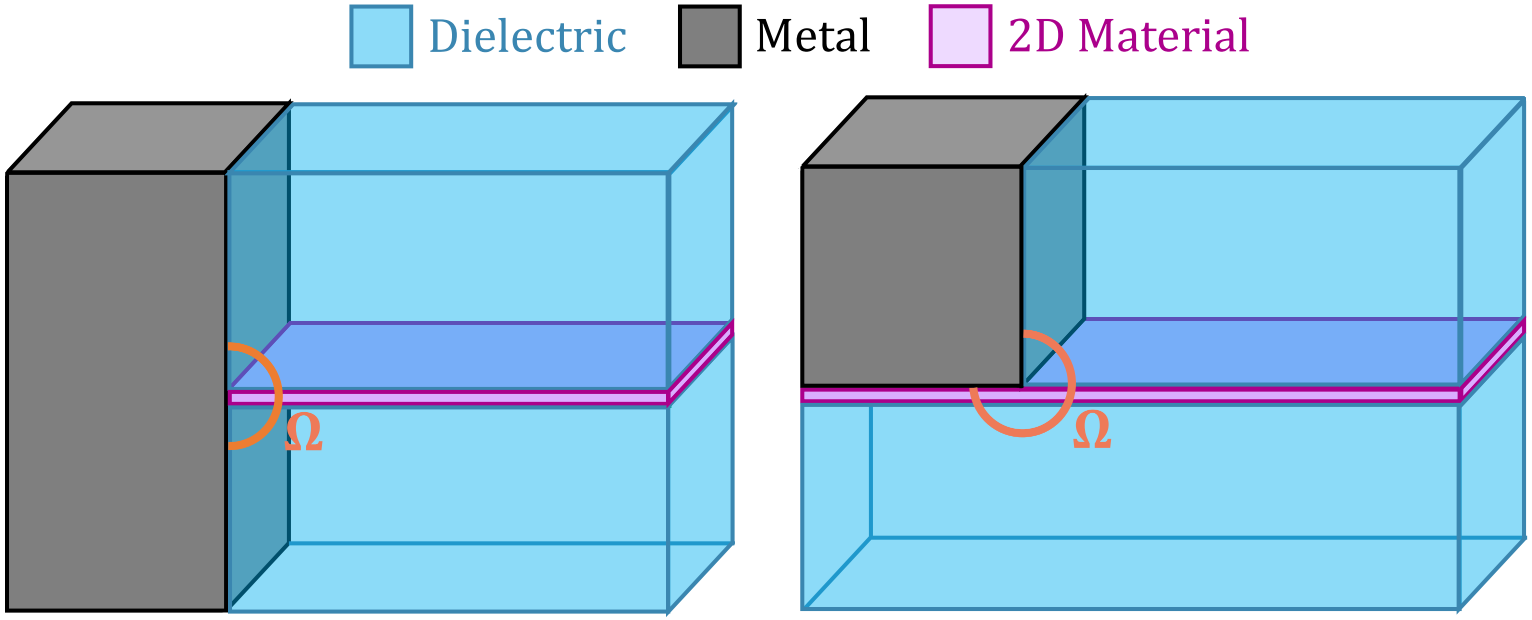
For asymmetrical geometry?



- ~~Method of images~~
- Poisson’s equation

The Problem:

- IFBL necessary to find R_C
- No solution for geometries like (b)

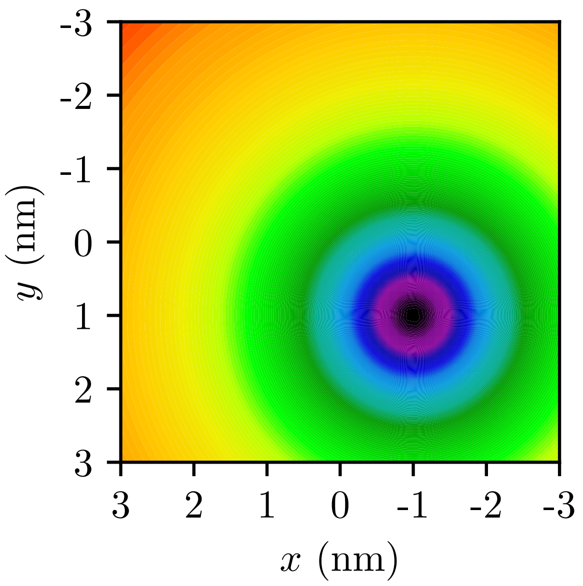


(a) $\Omega = \pi$ (b) $\Omega = 3\pi/2$

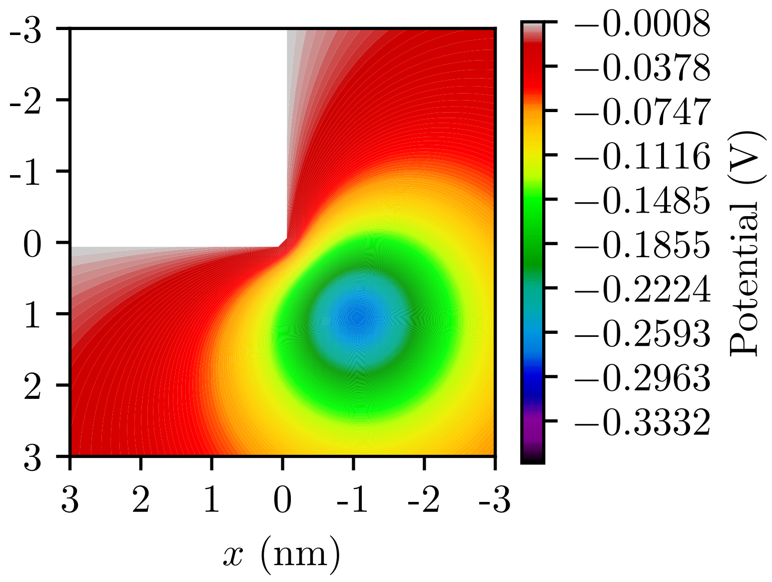
Isolating The Image Potential (V_I)

[3]

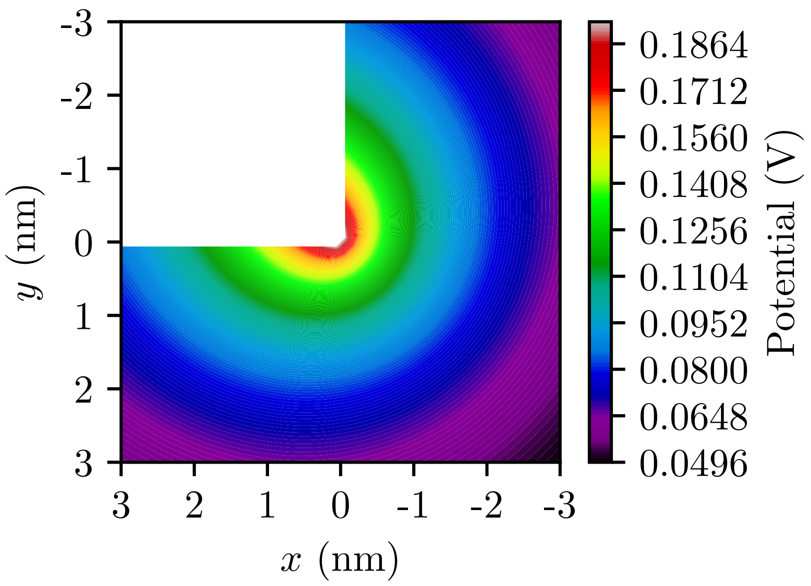
$$V_{\mathrm{I}} = V - V_{\mathrm{C}}$$



V_C



V



V_I

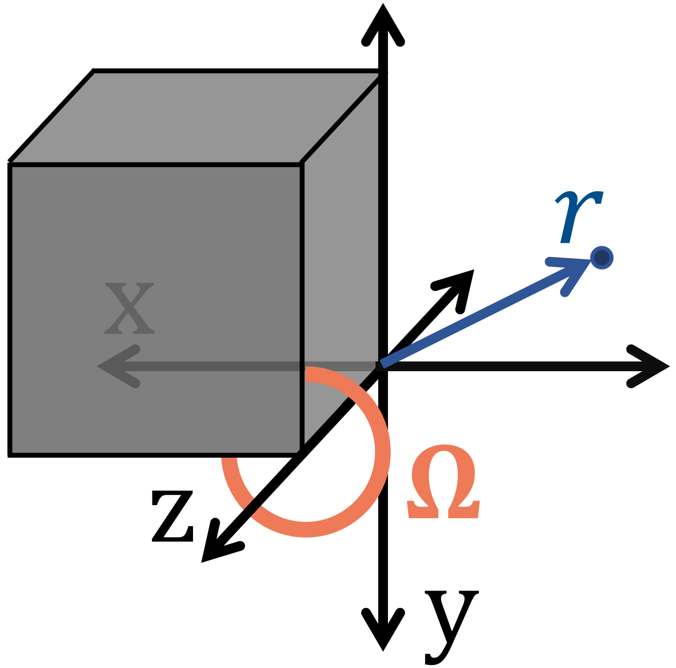
[3] S. Evans, *et al.*, “Image-Force Barrier Lowering for Two-Dimensional Materials: Direct Determination and Method of Images on a Cone Manifold,” arXiv, 2023

Determining U_{IFBL} from V_I

To find U_{IFBL}, we solve:

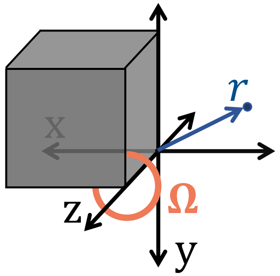
$$U_{\mathrm{IFBL}}(r,\theta) = -\int_0^{-e} \frac{q}{e} V_{\mathrm{I}}(r_0,\theta_0,z_0;r,\theta,z)\mathrm{d}q = -\frac{1}{2}eV_{\mathrm{I}}$$

Found from
$V_I = V – V_C$



q = charge of electron
e = charge of the electron inducing U_{IFBL}

Isolating V_I



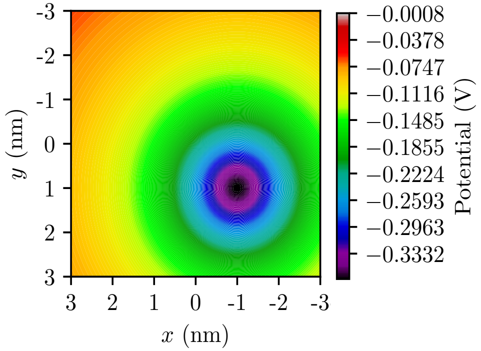
- Find V with Poisson's Equation:

$$V(r,\theta,z) = \frac{e}{\varepsilon}\int_0^\infty dk_z Z_{k_z}(z)\int_0^\infty d\alpha C_{\alpha,k_z}\Theta_\alpha(\theta)R_{\alpha k_z}(r)$$

  - Solve Θ(θ) with 2 sets of boundary conditions:

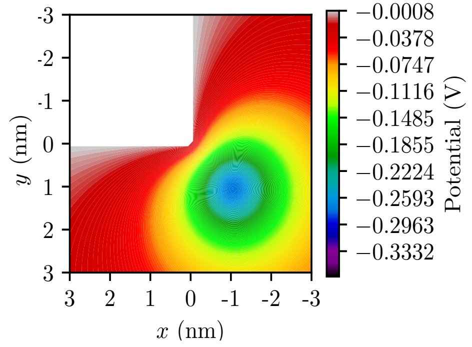
1. Point charge in free space (V_C)

$$\Theta_{C;\alpha}(\theta;\theta_0) = -\frac{\cosh(\alpha(\pi - |\theta - \theta_0|))}{\alpha\sinh(\alpha\pi)}$$



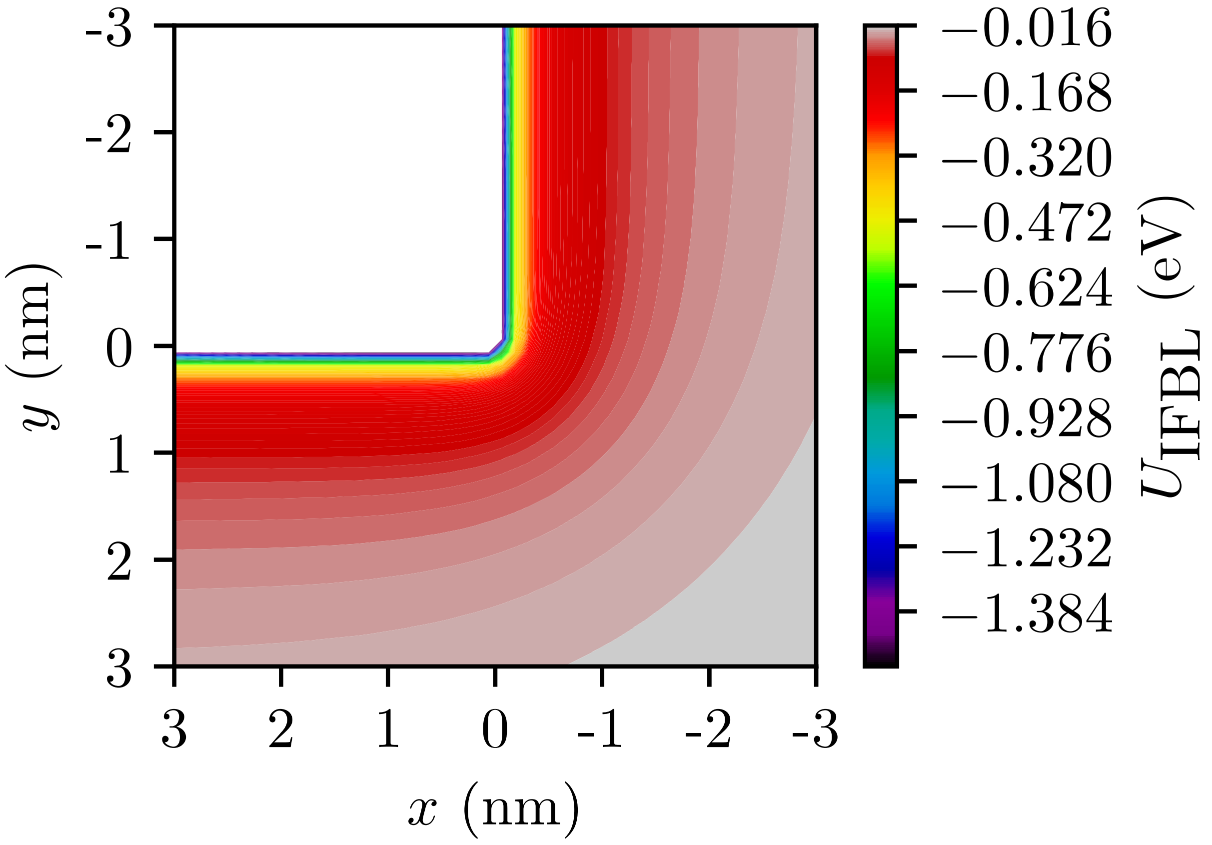
2. Point charge near a metal wedge (V)

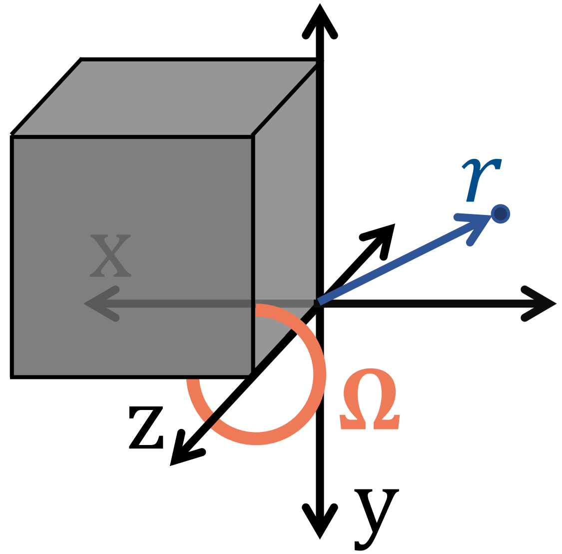
$$\Theta_{;\alpha}(\theta;\theta_0) = \frac{\sinh(\alpha\theta)\cosh\left(\alpha(\pi - (\Omega - \theta_0))\right)}{\alpha\sinh(\alpha\pi)\sinh(\alpha\Omega)} + \frac{\sinh(\alpha(\Omega - \theta))\cosh\left(\alpha(\pi - \theta_0)\right)}{\alpha\sinh(\alpha\pi)\sinh(\alpha\Omega)} - \frac{\cosh(\alpha(\pi - |\theta - \theta_0|))}{\alpha\sinh(\alpha\pi)}$$



Results: IFBL Potential Energy

$$U_{\mathrm{IFBL}}(r,\theta) = \frac{-e^2}{8\pi\epsilon r}\int_0^\infty \mathrm{d}\alpha\left(\frac{\sinh(\alpha\theta)\cosh(\alpha(\pi-(\Omega-\theta)))}{\sinh(\alpha\Omega)\cosh(\alpha\pi)} + \frac{\sinh(\alpha(\Omega-\theta))\cosh(\alpha(\pi-\theta))}{\sinh(\alpha\Omega)\cosh(\alpha\pi)}\right)$$



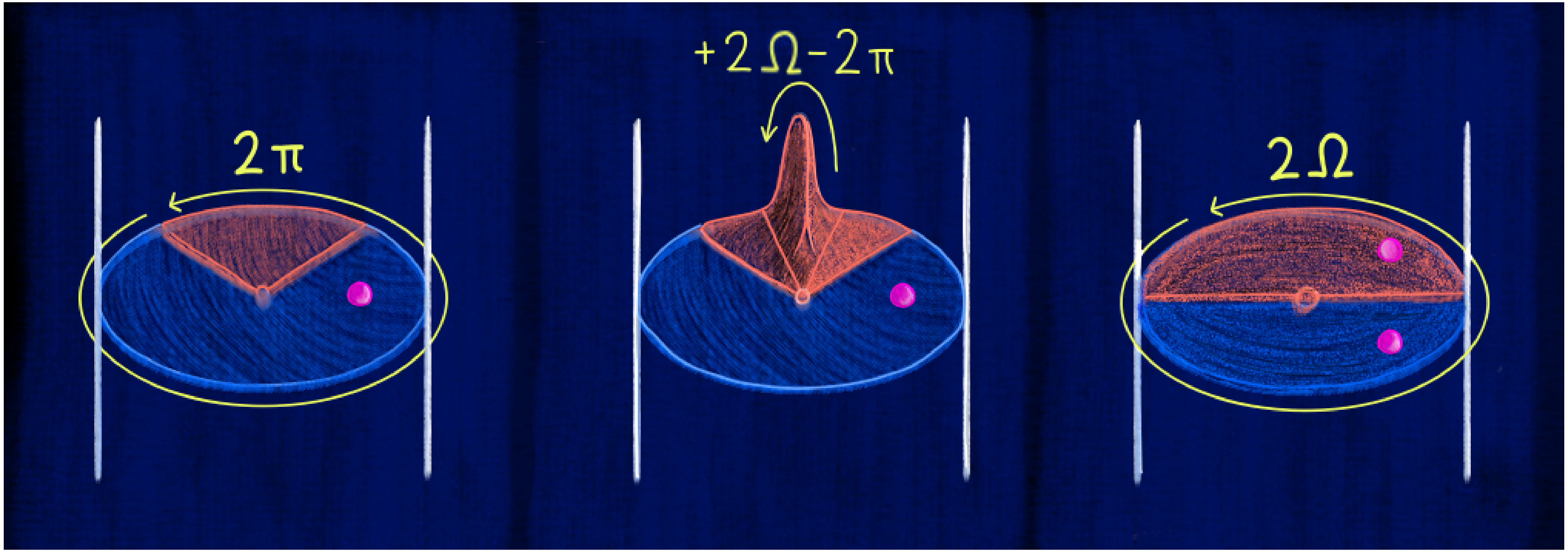


Method of Images on a Cone Manifold

Previously I said that I can not solve asymmetrical problems using method of images…

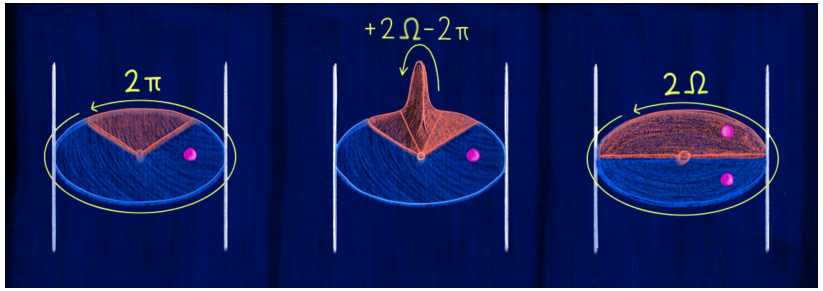
I LIED!

Method of Images on a Cone Manifold



Method of Images on a Cone Manifold (cont.)

- We can now **easily place an image charge**, regardless of asymmetrical geometry



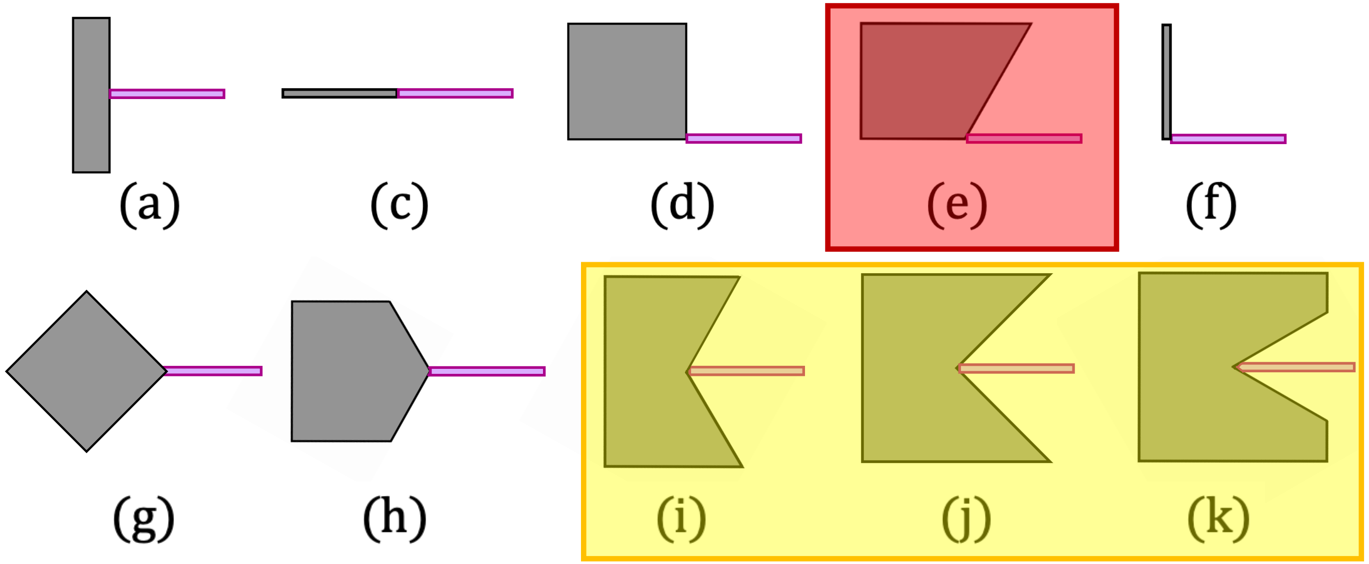
- Results are equal through trig identities

$$U_{\mathrm{IFBL}}(r,\theta)=\frac{-e^2}{8\pi\varepsilon r}\int_0^\infty \mathrm{d}\alpha\left(\frac{\cosh(\alpha(\Omega-\eta))\sinh(\alpha\pi)}{\sinh(\alpha\Omega)\cosh(\alpha\pi)}-\frac{\cosh(\alpha(\Omega-2\theta))\sinh(\alpha\pi)}{\sinh(\alpha\Omega)\cosh(\alpha\pi)}-\frac{\cosh(\alpha(\pi-\eta))}{\cosh(\alpha\pi)}\right)$$

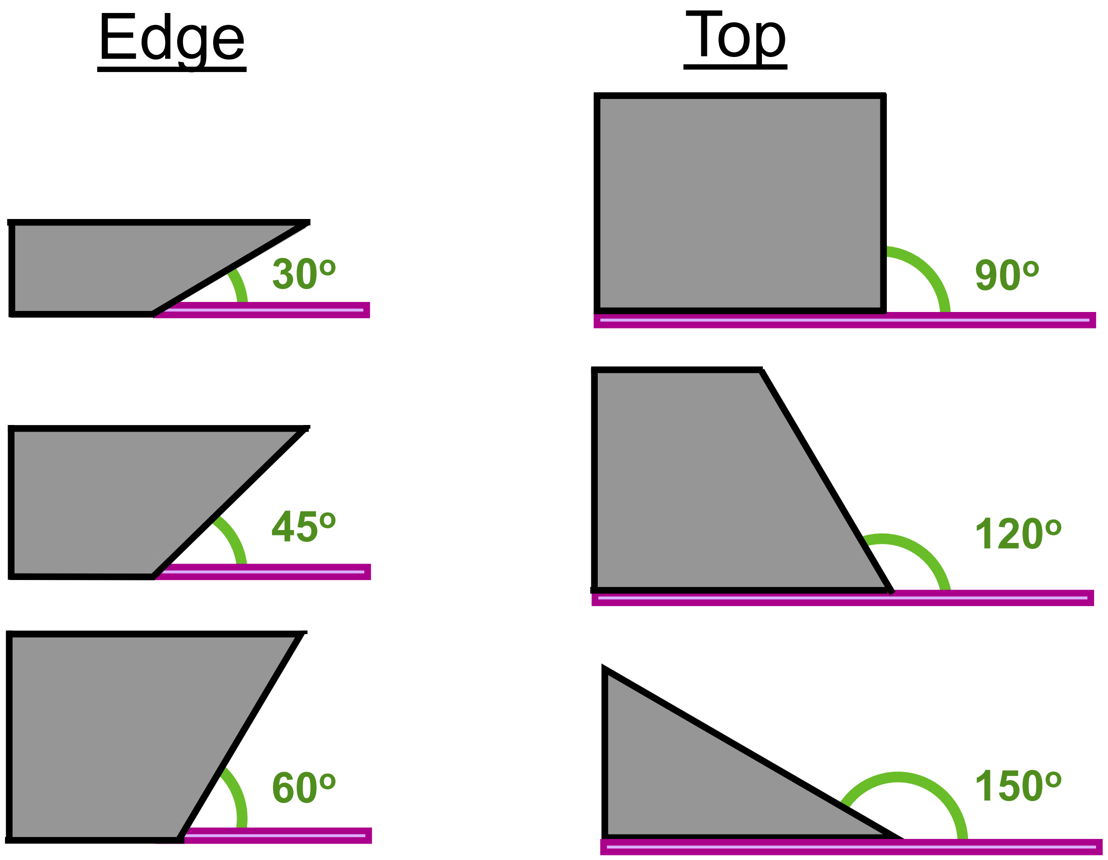
$$U_{\mathrm{IFBL}}(r,\theta)=\frac{-e^2}{8\pi\varepsilon r}\left(\int_0^\infty \mathrm{d}\alpha\frac{\sinh(\alpha(\Omega-\pi))}{\sinh(\alpha\Omega)\cosh(\alpha\pi)}+\int_0^\infty \mathrm{d}\alpha\frac{\cosh(\alpha(\Omega-2\theta))\tanh(\alpha\pi)}{\sinh(\alpha\Omega)}\right)$$

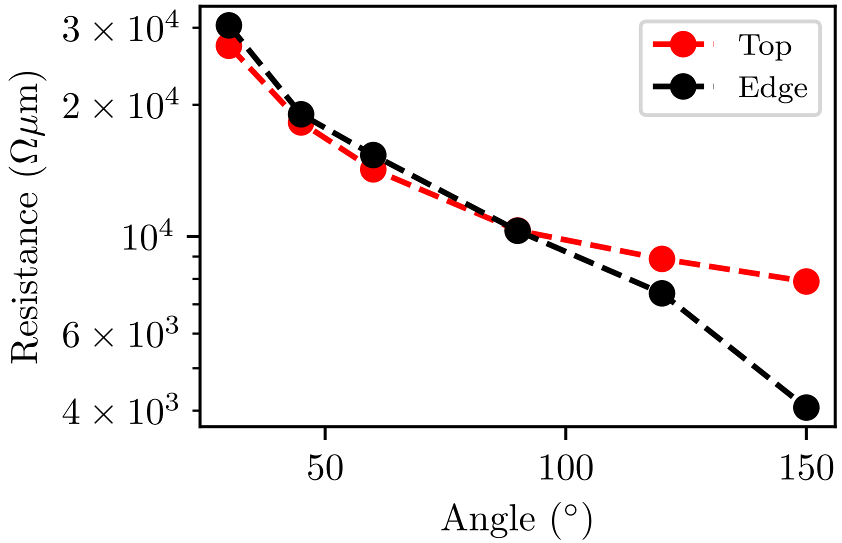
Results: U_{IFBL}

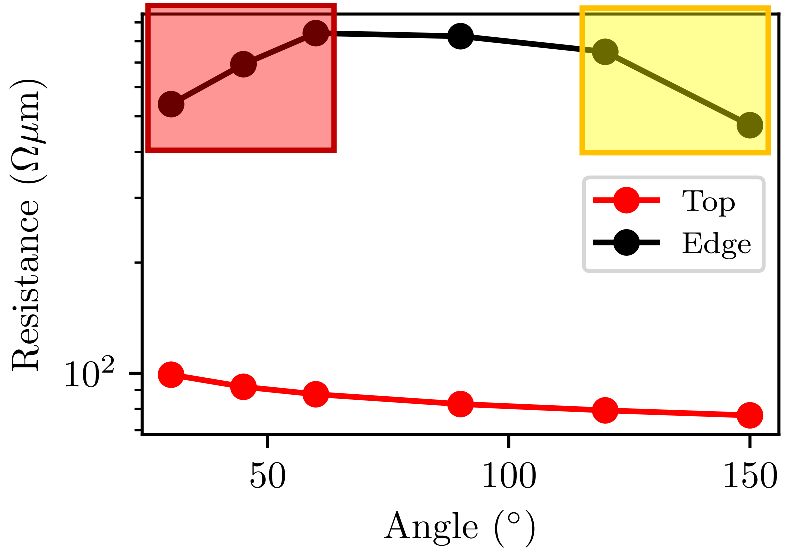
	Ω	θ	$U_{IFBL}/(-e^2/(16\pi\varepsilon r))$
a	π	$\pi/2$	1
b	π	θ	$\csc(\theta)$
c	2π	π	0.63
d	$3\pi/2$	π (or $\pi/2$)	0.85
e	$4\pi/3$	π	1.11
f	2π	$3\pi/2$	0.82
g	$3\pi/2$	$\Omega/2 = 3\pi/4$	0.74
h	$4\pi/3$	$\Omega/2 = 2\pi/3$	0.81
i	$2\pi/3$	$\Omega/2 = \pi/3$	1.41
j	$\pi/2$	$\Omega/2 = \pi/4$	1.83
k	$\pi/3$	$\Omega/2 = \pi/6$	2.69



Results: Contact Resistance







Conclusions

- IFBL necessary for accurate R_C calculation
  - But significantly impacted by contact geometry

- U_{IFBL} determined for asymmetrical geometries:
  - Poisson's equation
  - Cone manifold

- $U_{\mathrm{IFBL}} \propto \frac{1}{\epsilon}$

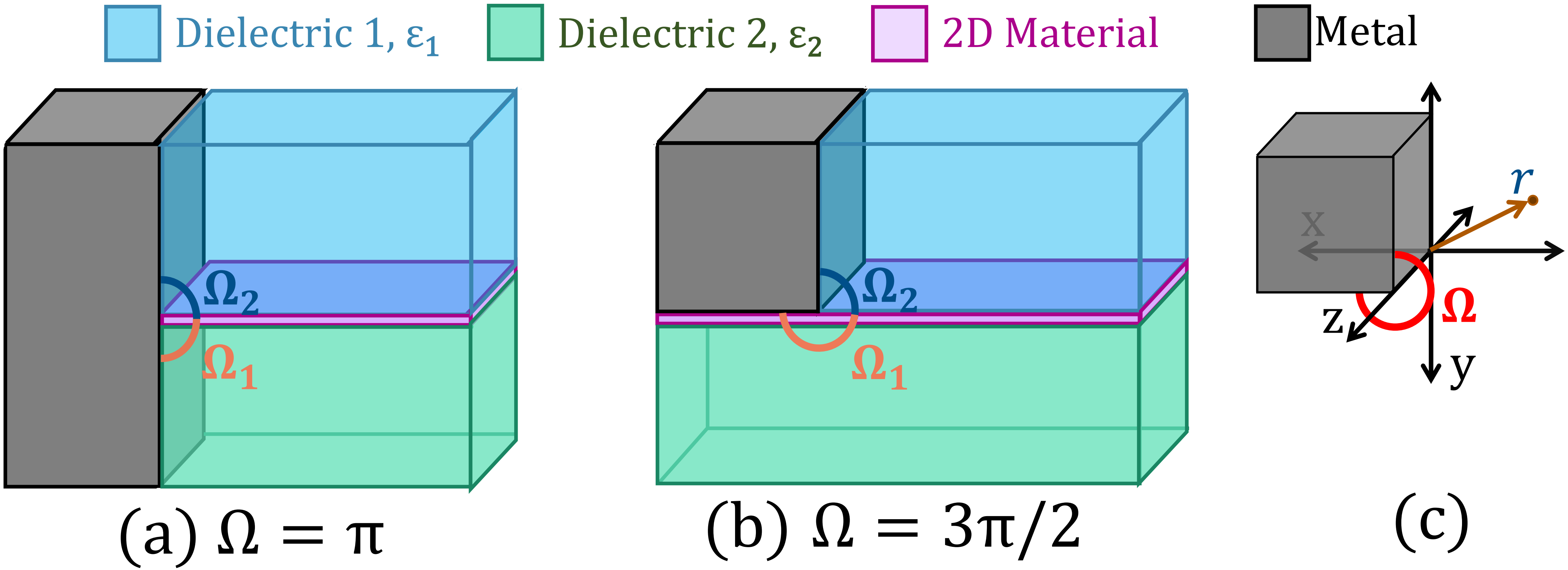
- Contact angle can act as tunable parameter
  - Impacts Schottky barrier and R_C

Thank you!

Please feel free to ask any questions

S. Evans, *et al.*, "Image-Force Barrier Lowering for Two-Dimensional Materials: Direct Determination and Method of Images on a Cone Manifold," arXiv, 2023

Future work


Dielectric 1, ε_1
Dielectric 2, ε_2
2D Material
Metal
Ω_2
Ω_1
Ω_2
Ω_1
x
z
y
r
Ω
(a) $\Omega = \pi$
(b) $\Omega = 3\pi/2$
(c)

$$U_{\mathrm{IFBL}}(r,\theta) = -\int_0^{-e} \frac{q}{e} V_{\mathrm{I}}(r_0,\theta_0,z_0;r,\theta,z)\mathrm{d}q = -\frac{1}{2}eV_{\mathrm{I}} \quad (1)$$

$$\Theta_{\mathrm{I};\alpha}(\theta;\theta_0) = \frac{\sinh(\alpha\theta)\cosh\left(\alpha(\pi-(\Omega-\theta_0))\right)}{\alpha\sinh(\alpha\pi)\sinh(\alpha\Omega)} + \frac{\sinh(\alpha(\Omega-\theta))\cosh\left(\alpha(\pi-\theta_0)\right)}{\alpha\sinh(\alpha\pi)\sinh(\alpha\Omega)} \quad (2)$$

$$\Theta_{\mathrm{C};\alpha}(\theta;\theta_0) = -\frac{\cosh(\alpha(\pi-|\theta-\theta_0|))}{\alpha\sinh(\alpha\pi)} \quad (3)$$

$$V_{\mathrm{I}} = \frac{e}{4\pi\epsilon\sqrt{rr_0}}\int_0^{\infty}\mathrm{d}\alpha P_{i\alpha-1/2}\left(\frac{(z-z_0)^2+r_0^2+r^2}{2rr_0}\right) \quad (4)$$
$$\left(\frac{\sinh(\alpha\theta)\cosh\left(\alpha(\pi-(\Omega-\theta_0))\right)}{\sinh(\alpha\Omega)\cosh(\alpha\pi)} + \frac{\sinh(\alpha(\Omega-\theta))\cosh\left(\alpha(\pi-\theta_0)\right)}{\sinh(\alpha\Omega)\cosh(\alpha\pi)}\right)$$

$$\Theta^{\circledast}_{\mathrm{C};\alpha}(\theta;\theta_0) = -\frac{\cosh(\alpha(\Omega-|\theta-\theta_0|))}{\alpha\sinh(\alpha\Omega)} \quad (6)$$

$$U_{\mathrm{IFBL}}(r,\theta) = \frac{-e^2}{8\pi\epsilon r}\int_0^{\infty}\mathrm{d}\alpha\left(\frac{\sinh(\alpha\theta)\cosh(\alpha(\pi-(\Omega-\theta)))}{\sinh(\alpha\Omega)\cosh(\alpha\pi)} + \frac{\sinh(\alpha(\Omega-\theta))\cosh(\alpha(\pi-\theta))}{\sinh(\alpha\Omega)\cosh(\alpha\pi)}\right) \quad (5)$$

$$U_{\mathrm{IFBL}}(r,\theta) = \frac{-e^2}{8\pi\epsilon r}\int_0^{\infty}\mathrm{d}\alpha\frac{\cosh(\alpha(\Omega-2\theta))\sinh(\alpha\pi)+\sinh(\alpha(\Omega-\pi))}{\sinh(\alpha\Omega)\cosh(\alpha\pi)} \quad (7)$$