Theoretical (Computational) Symposium

on Atomic Collisions in Solids

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EXTENSIONS TO THE TWO ATOM BLOCKING MODEL

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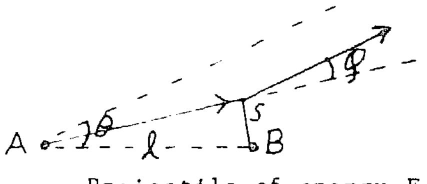
EXTENSIONS TO THE TWO ATOM BLOCKING MODEL

Blocking Model

Widely used to interpret blocking and surface scattering experiments.

Shadow cones
Surface structure
Aono experiments
Nuclear lifetimes
Backward glory effect — 180° enhanced backscattering

Ingredients c Model



Projectile of energy E starts at atom A and is scattered by atom B

1. Classical scattering theory
2. Impulse approximation
3. Thermal displacements included

ATTRACTIVE POTENTIAL

BLOCKING ⟶ FOCUSSING

$$\theta = \frac{s}{\ell} - \phi(s)$$

Normalized differential scattering cross section per unit solid angle is

$$F_A(\theta) = \frac{1}{\ell^2} \left| \frac{s}{\theta} \right| \frac{ds}{d\theta}$$

for Coulomb potential

$$\phi(s) = b/s \;, \qquad b = \frac{Z_1 Z_2 e^2}{E}$$

$$\theta^* = 0.5 \left(s^* - \frac{1}{s^*} \right) \qquad \text{where}$$

$$\theta^* = \frac{\theta}{\theta_c} \;, \quad \theta_c = 2\sqrt{b/\ell} \;, \quad s^* = \frac{s}{s_c} \;, \quad s_c = \sqrt{b\ell}$$

$$F_A = \frac{1}{2} \left\{ \frac{\sqrt{\theta^{*2}+1}}{\theta^*} + \frac{\theta^*}{\sqrt{\theta^{*2}+1}} \right\} \quad |\theta^*| > 0$$

$$F_R = \frac{1}{2} \left\{ \frac{\sqrt{\theta^{*2}-1}}{\theta^*} + \frac{\theta^*}{\sqrt{\theta^{*2}-1}} \right\} \quad |\theta^*| > \theta_c$$

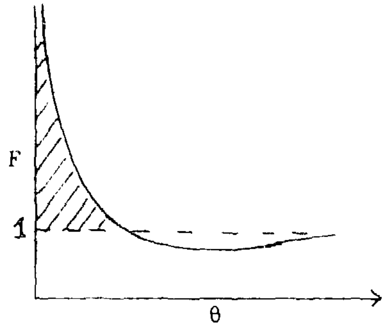
SOME OBSERVATIONS

1. For attractive potential, the singularity in the scattering pattern occurs when $\theta^* = 0$.

2. For attractive case, some $+\theta^*$ come from negative s^*, for Coulomb scattering the separation occurs when $s^* = 1$ or $s = \sqrt{b\ell}$.

3. The equation giving the attractive Coulomb scattering pattern is the same as for repulsive Coulomb except for the sign within the radical.

Compensation ?



$$G = 2\pi \int_0^{\theta_m} [F(\theta) - 1]\theta d\theta$$

$$= \pi \left[\frac{s_u^2}{\ell^2} - \frac{s_\ell^2}{\ell^2} - \theta_m^2\right]$$

for arbitrary potential

$$= \pi \left[\frac{s_u^2}{\ell^2} - \frac{s_\ell^2}{\ell^2} - \frac{s_u^2}{\ell^2} + \frac{2 s_u \phi_u}{\ell} - \phi_u^2\right] \Big\} \to 0$$

Provided $\phi \to 0$ faster than Coulomb

$$= \frac{\pi 2b}{\ell} = \frac{\pi \theta_c^2}{2}$$ for Coulomb

Two particle emission for attractive (repulsive) potential

$$F(\theta) \int_0^\infty \frac{2sds}{\langle\rho^2\rangle} \exp^{-\left[\frac{(\ell\theta)^2+(s\pm\ell\phi)^2}{\langle\rho^2\rangle}\right]} I_o\left[\frac{2\ell\theta(s\pm\ell\phi)}{\langle\rho^2\rangle}\right]$$

- attractive

+ repulsive

ρ is relative thermal displacement

I_o is modified Bessel function of 1st kind

$$F(0) = 2 \int_0^\infty \frac{sds}{\langle\rho^2\rangle} \exp\left[-\frac{(s\pm\ell\phi)^2}{\langle\rho^2\rangle}\right]$$

Specializing to Coulomb potential

$$F(\theta) = \eta \exp(-\alpha \pm \eta) \sum_{k=0}^{\infty} f_k \qquad \begin{matrix} - F_R \\ + F_A \end{matrix}$$

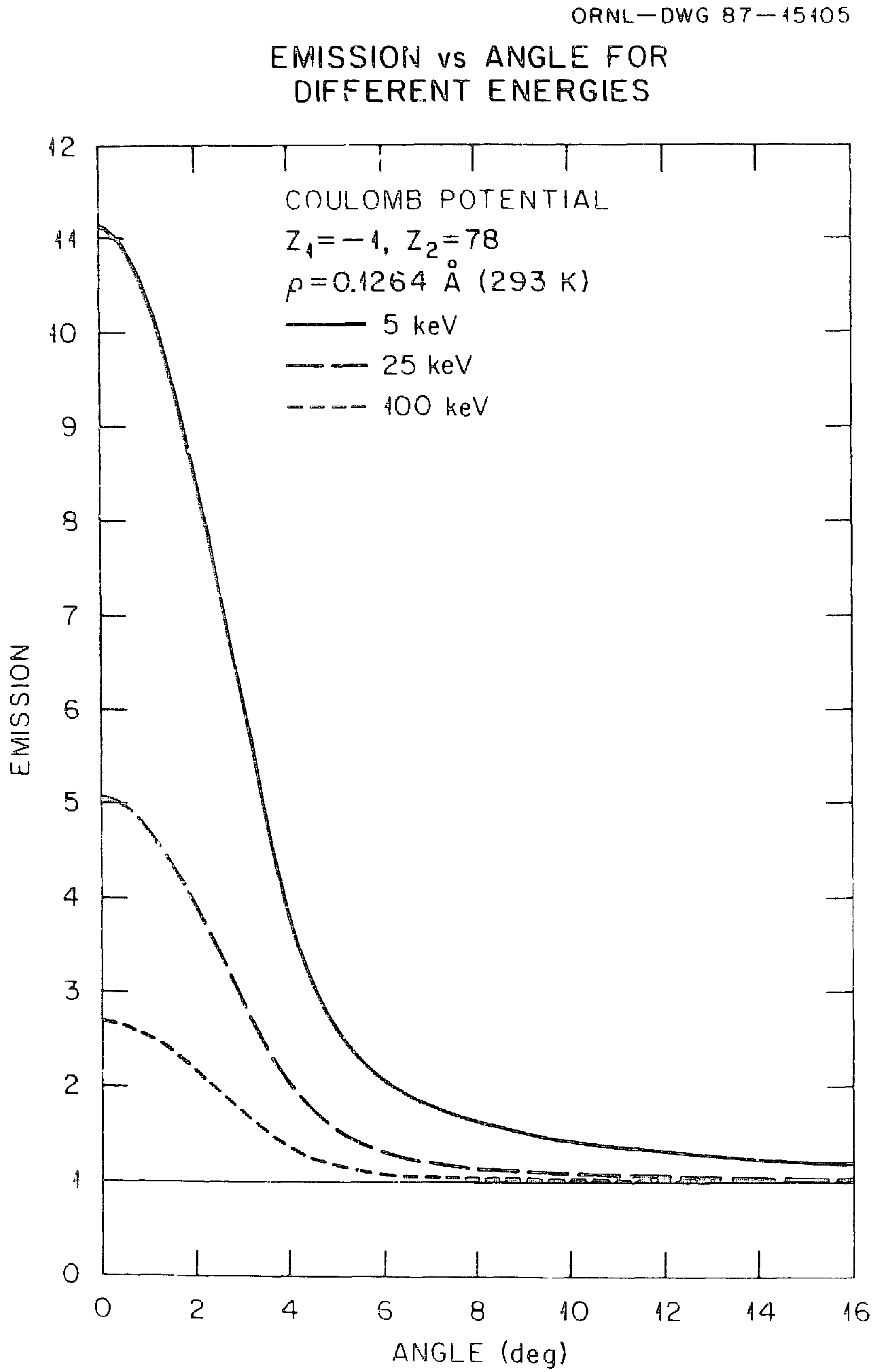
where $\alpha = \dfrac{(\ell\theta)^2}{\langle p^2 \rangle}$, $\eta = \dfrac{\theta_c^2 \ell^2}{2\langle p^2 \rangle}$

$$f_k = \left(\frac{\alpha\eta}{2}\right)^k \frac{g_k}{(k!)^2}$$

$$g_k = \sum_{r=0}^{2k} \frac{(\mp 1)^r (2k)!}{(2k-r)!\,r!} K_{r+1-k}(\eta)$$

K_r is modified Bessel fcn. of 3rd kind

$$F(0) = \eta \exp(-\alpha \pm \eta) K_1(\eta)$$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EMISSION vs ANGLE FOR DIFFERENT ENERGIES
COULOMB POTENTIAL
Z1=−1, Z2=78
ρ=0.1264 Å (293 K)
5 keV
25 keV
100 keV
EMISSION
ANGLE (deg)
0
1
2
3
4
5
6
7
8
9
10
11
12
0
2
4
6
8
10
12
14
16

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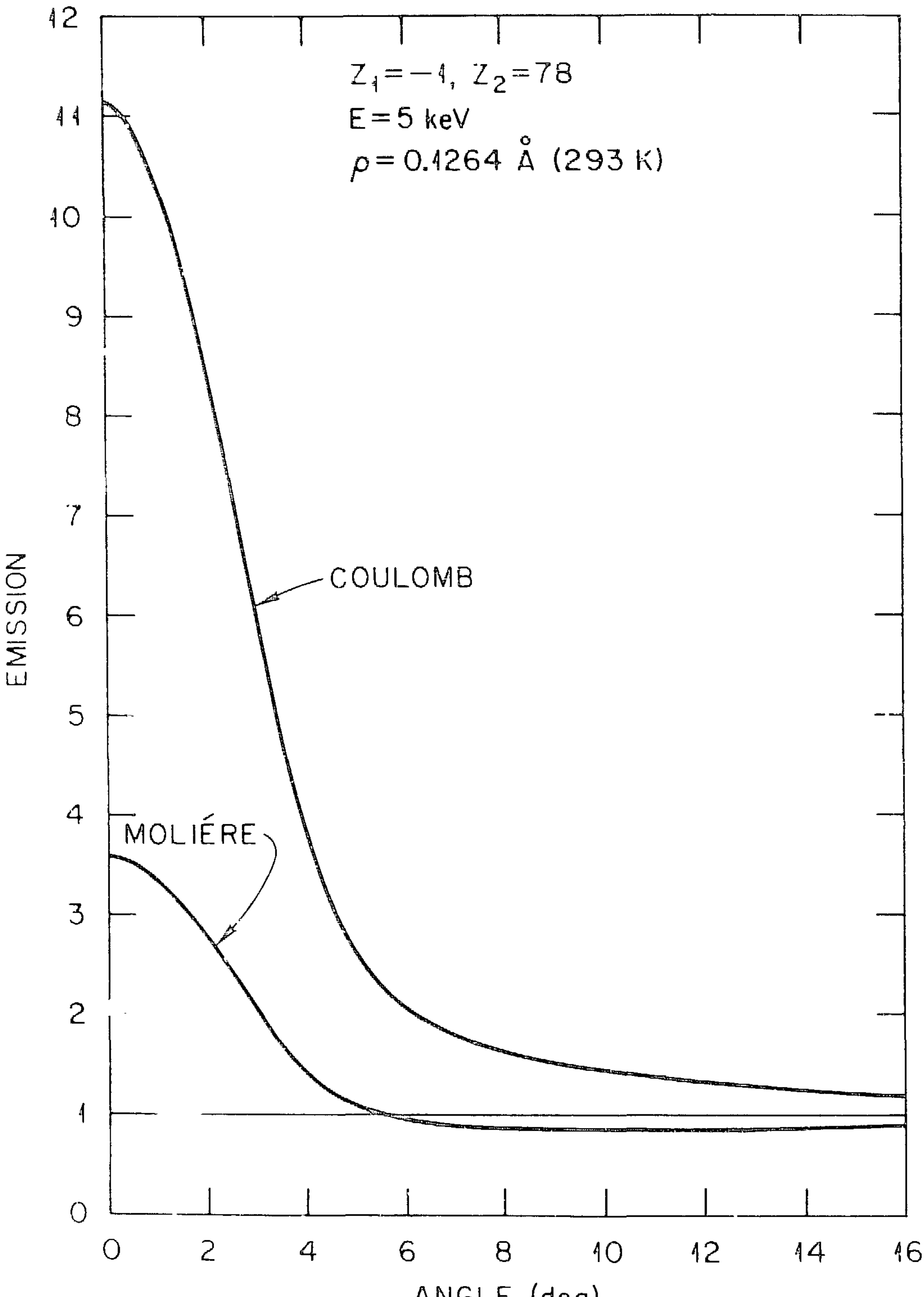
EMISSION vs ANGLE FOR MOLIÉRE AND COULOMB SCATTERING



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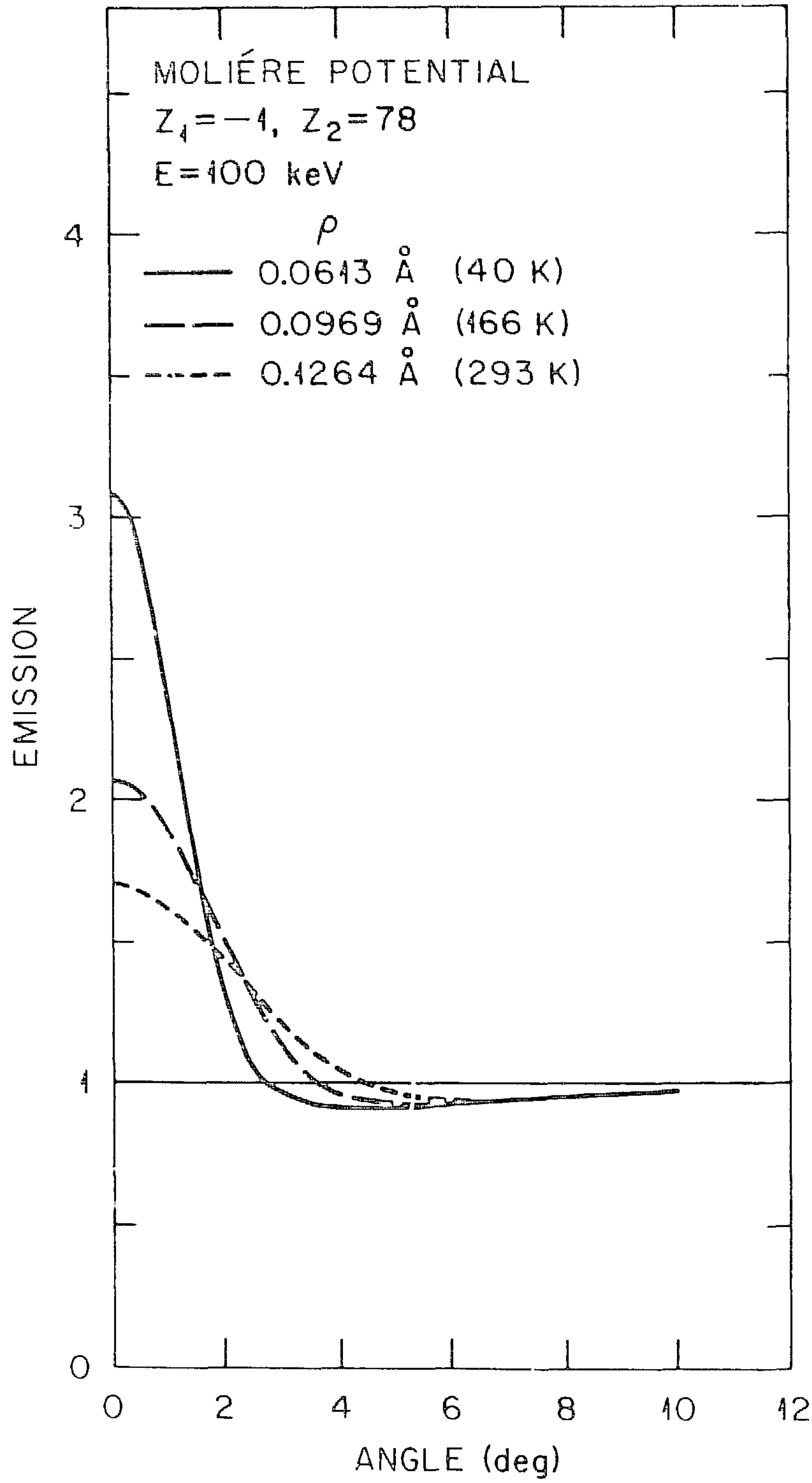
EMISSION vs ANGLE FOR DIFFERENT TEMPERATURES



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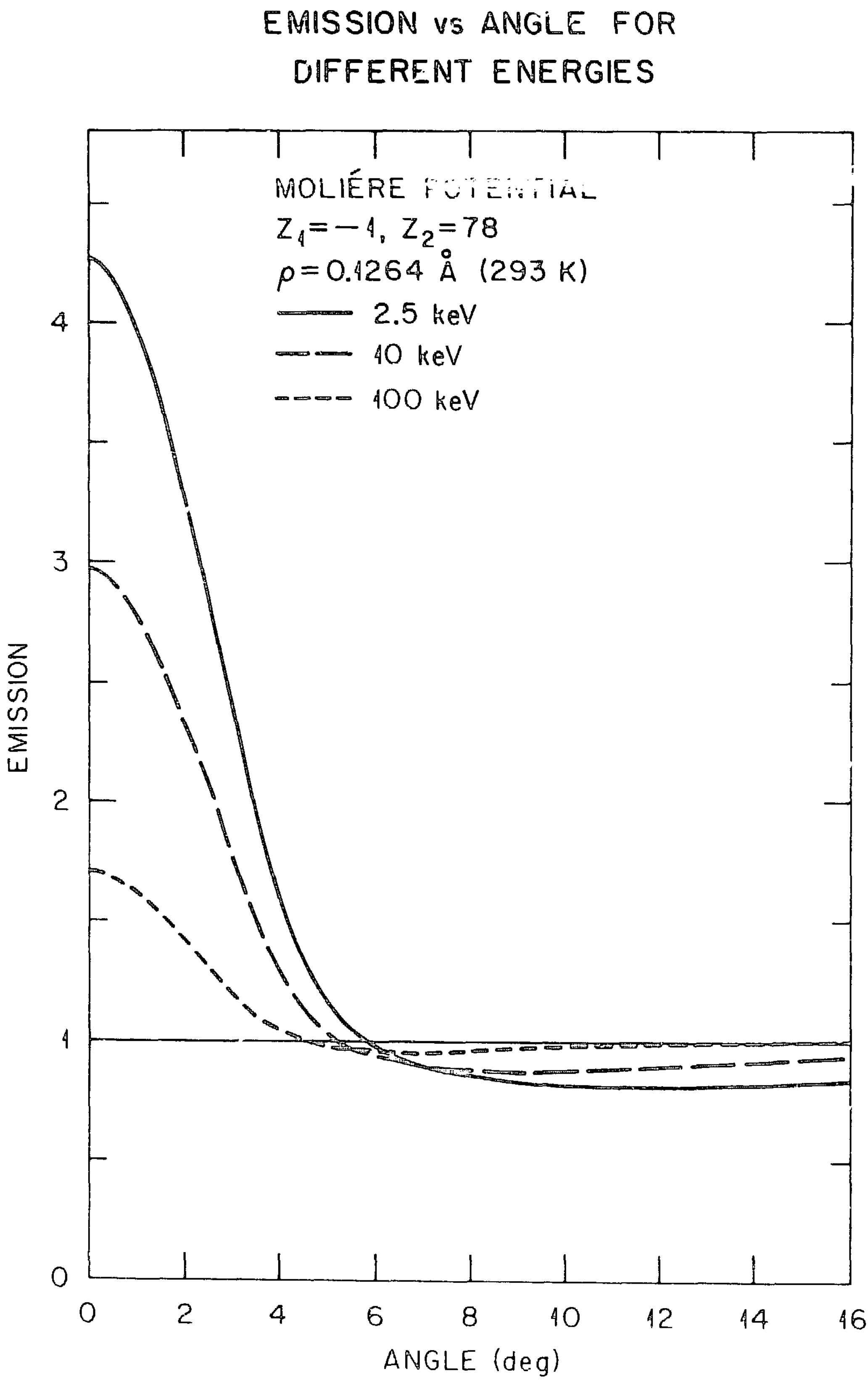

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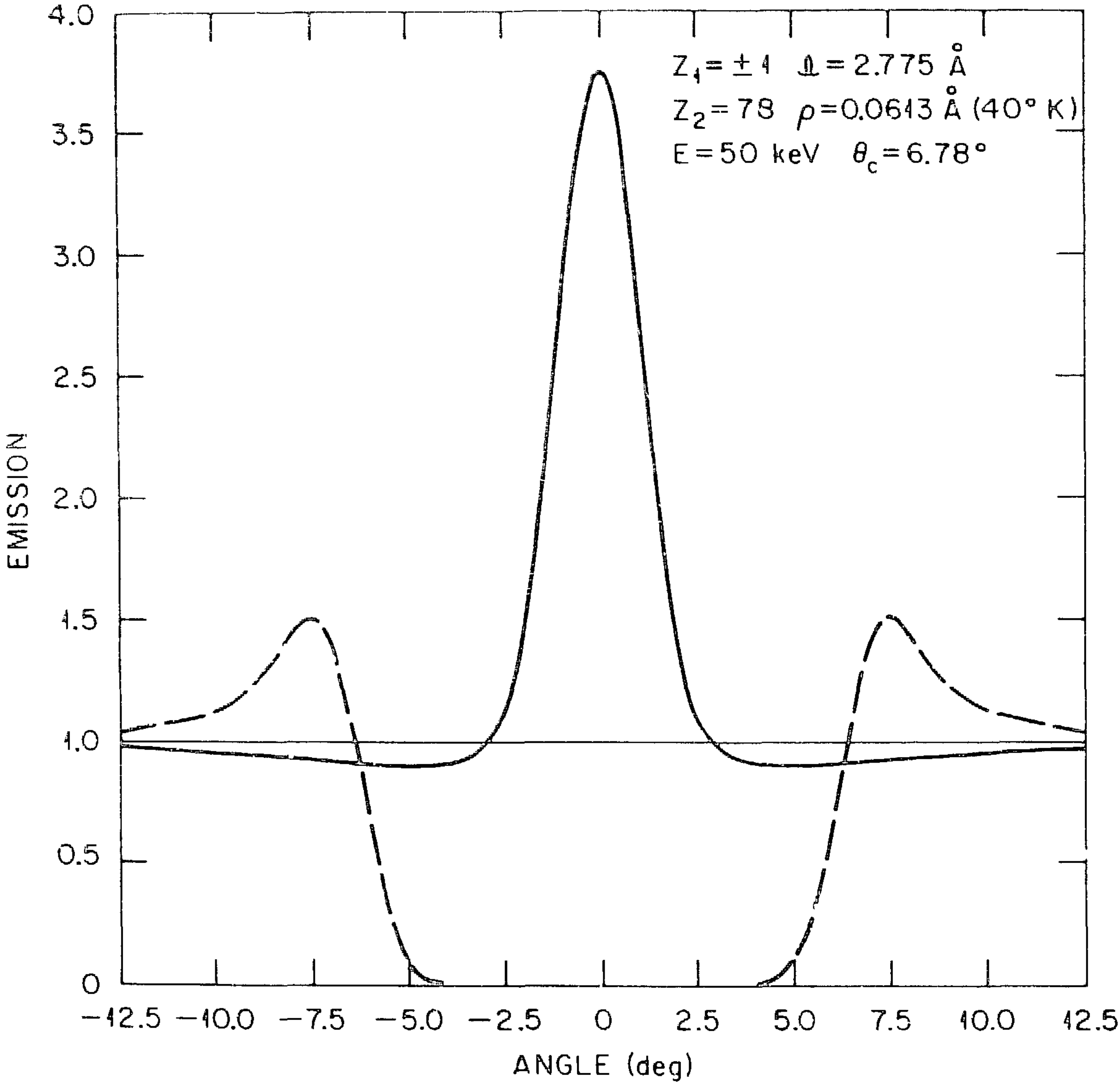
EMISSION vs ANGLE FOR ATTRACTIVE AND REPULSIVE MOLIÉRE POTENTIALS



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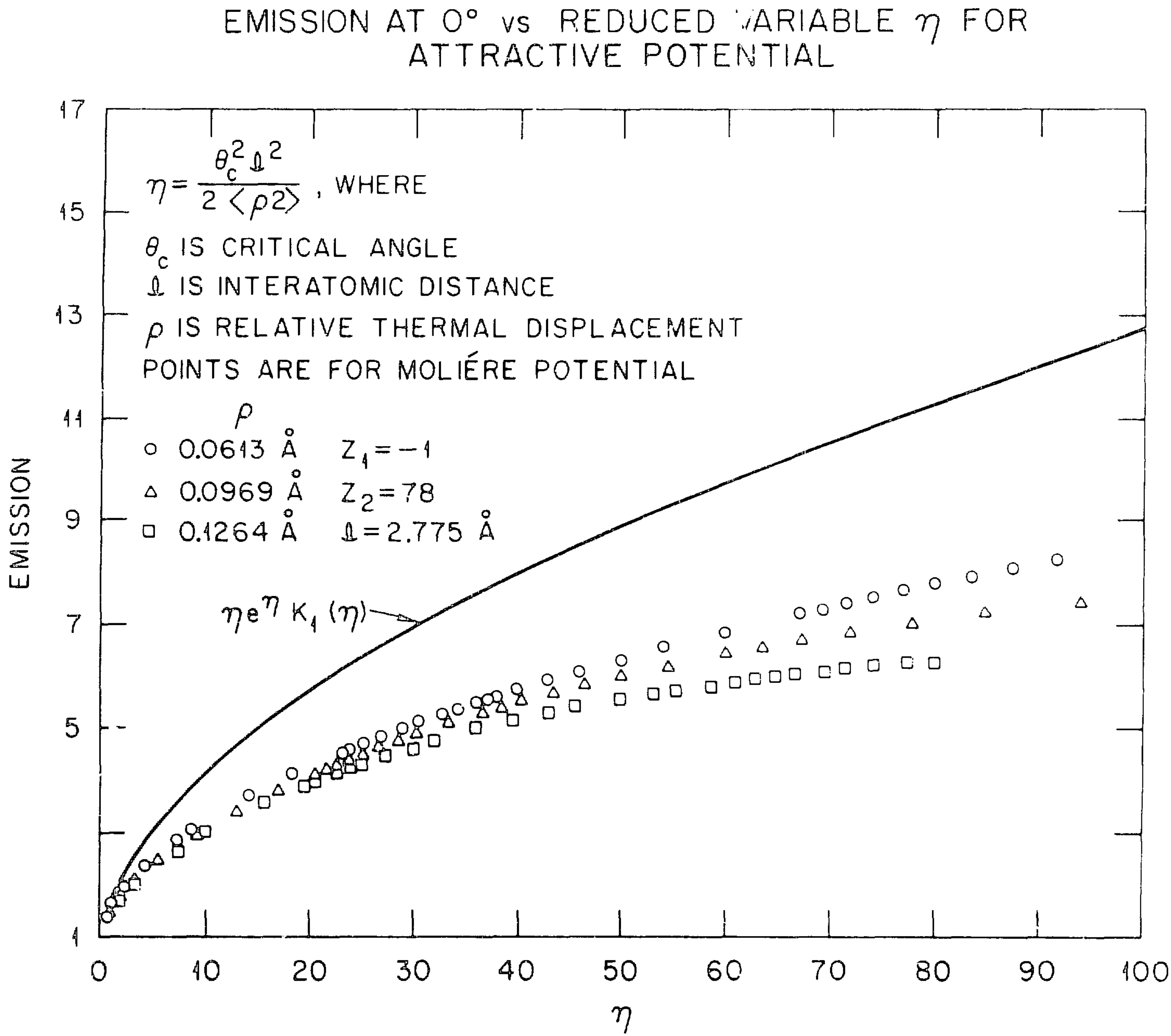

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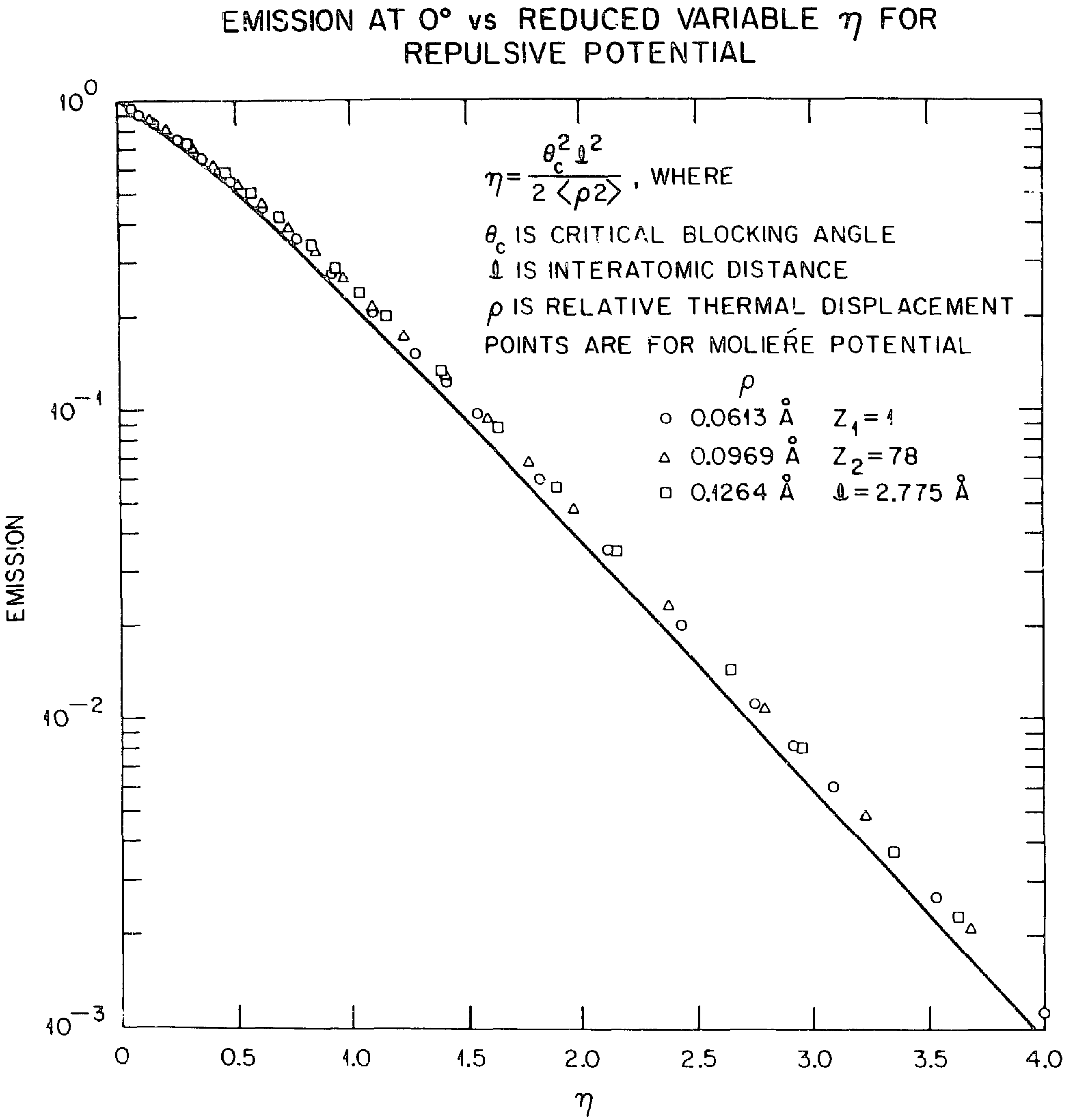

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EMISSION vs REDUCED ANGLE

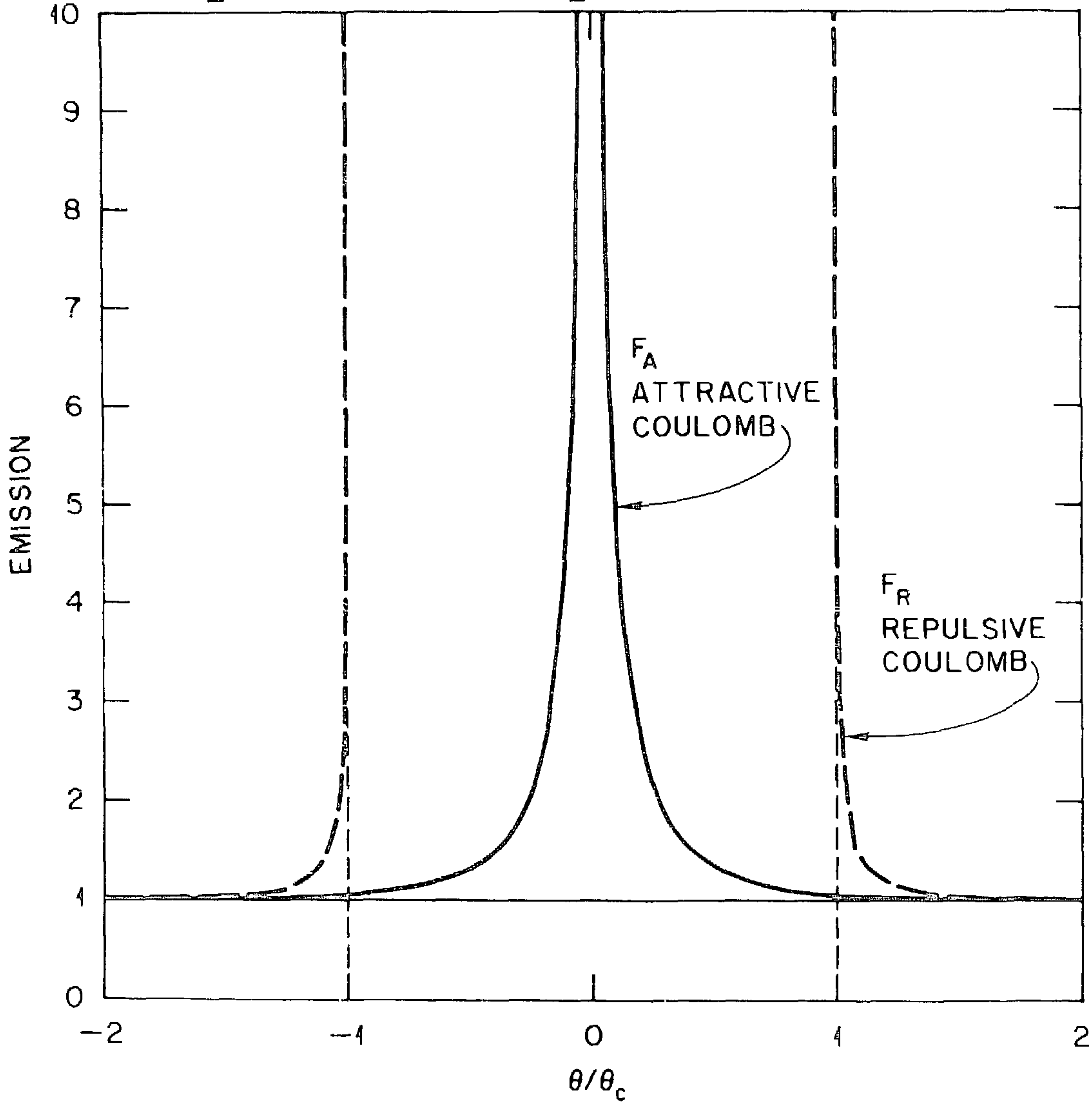
$$F_R = 1/2\left[\left(1-\frac{\theta_c^2}{\theta^2}\right)^{1/2} + \left(1-\frac{\theta_c^2}{\theta^2}\right)^{-1/2}\right]$$

$$F_A = 1/2\left[\left(1+\frac{\theta_c^2}{\theta^2}\right)^{1/2} + \left(1+\frac{\theta_c^2}{\theta^2}\right)^{-1/2}\right]$$

$$\theta_c = 2\sqrt{\frac{Z_1 Z_2 e^2}{\ell E}}$$

E = ENERGY

ℓ = DISTANCE BETWEEN ATOMIC CENTERS



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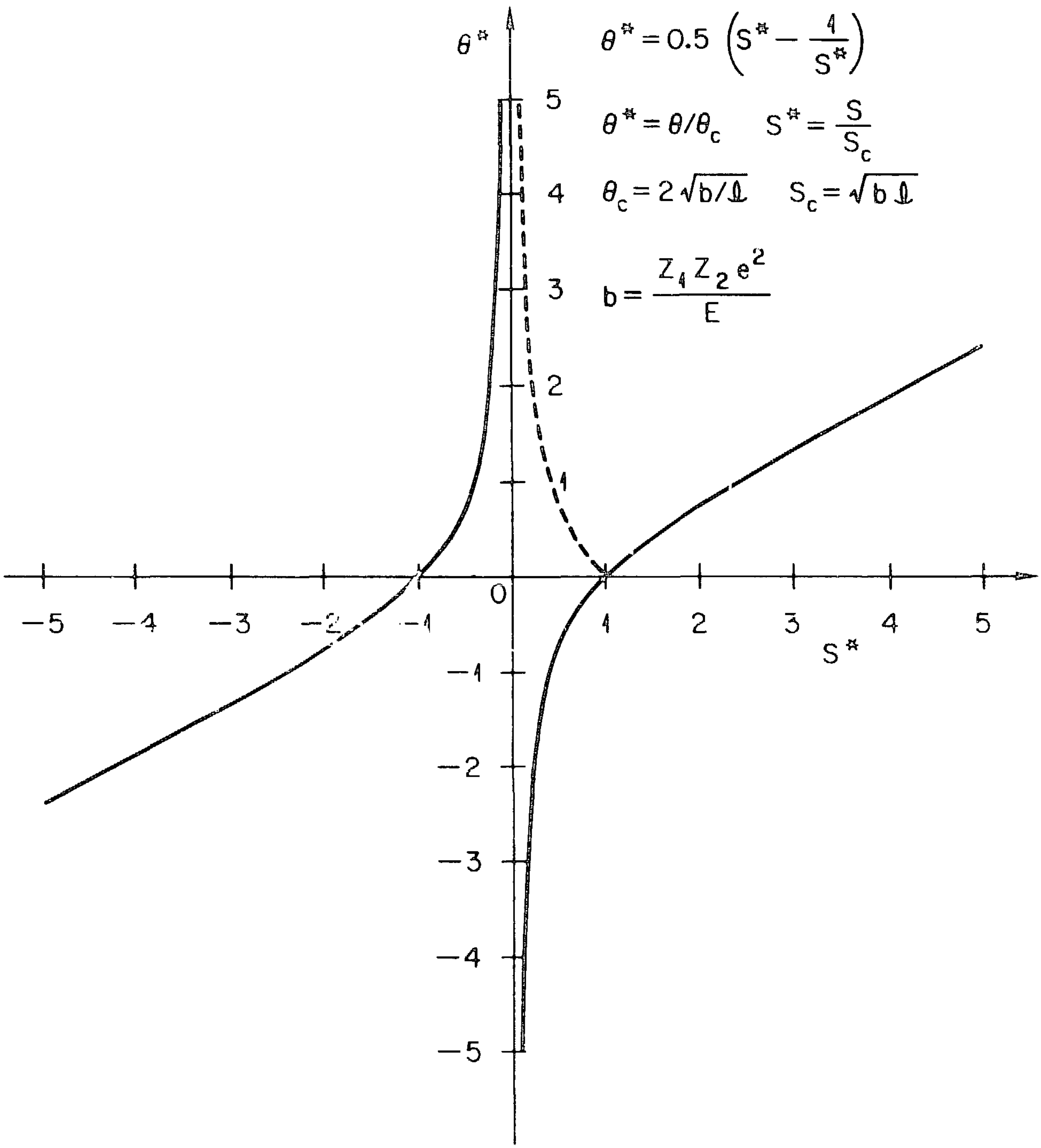
REDUCED DEVIATION ANGLE θ^* vs REDUCED IMPACT PARAMETER S^* (ATTRACTIVE COULOMB POTENTIAL)



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REDUCED DEVIATION ANGLE θ^* vs REDUCED IMPACT PARAMETER S^* (REPULSIVE COULOMB POTENTIAL)

$$\theta^* = 0.5\left(S^* + \frac{1}{S^*}\right)$$

$$\theta^* = \theta/\theta_c \qquad S^* = \frac{S}{S_c}$$

$$\theta_c = 2\sqrt{b/\ell} \qquad S_c = \sqrt{b\,\ell}$$

$$b = \frac{Z_1 Z_2 e^2}{E}$$