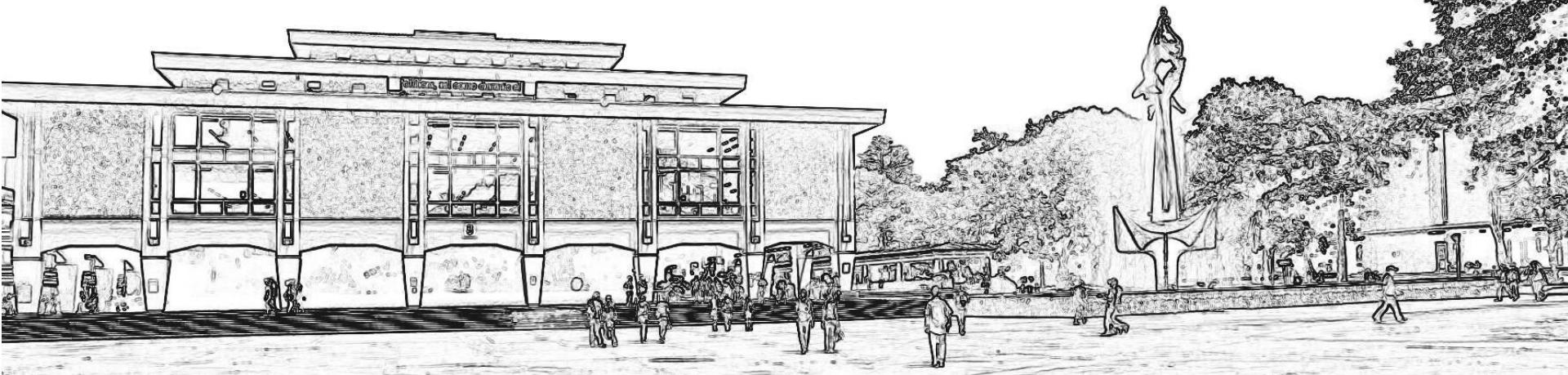




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Simulación numérica de dispersión potencial de

Por: Alejandro Restrepo, Carlos Granada y Sebastián Ramirez

$$AX(n,n)$$

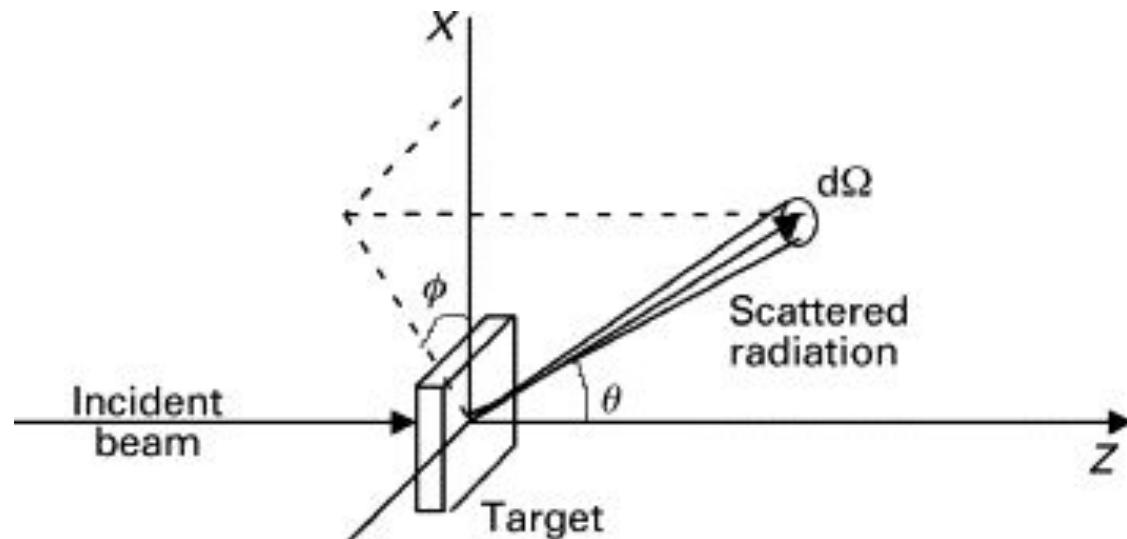


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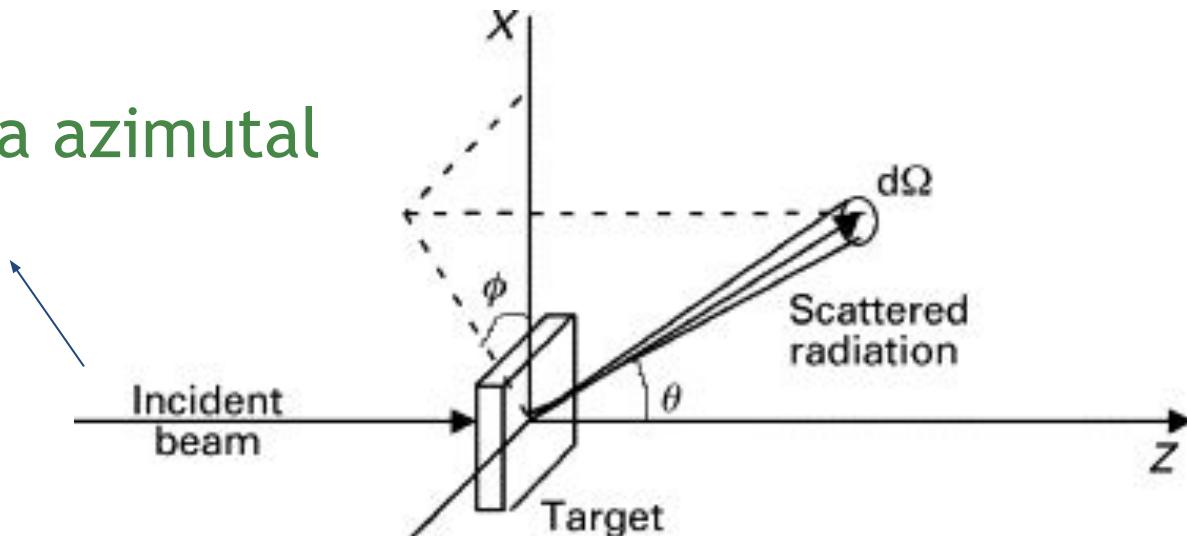
Planteamiento del problema

Problema de la dispersión



Problema de la dispersión

Simetría azimutal



Nos interesa conocer

$$\frac{d\sigma}{d\Omega}(\theta)$$

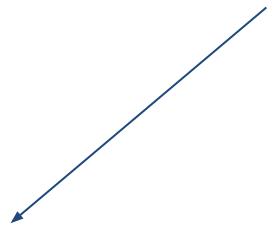
: Flujo saliente por unidad de ángulo sólido, por unidad de flujo incidente.



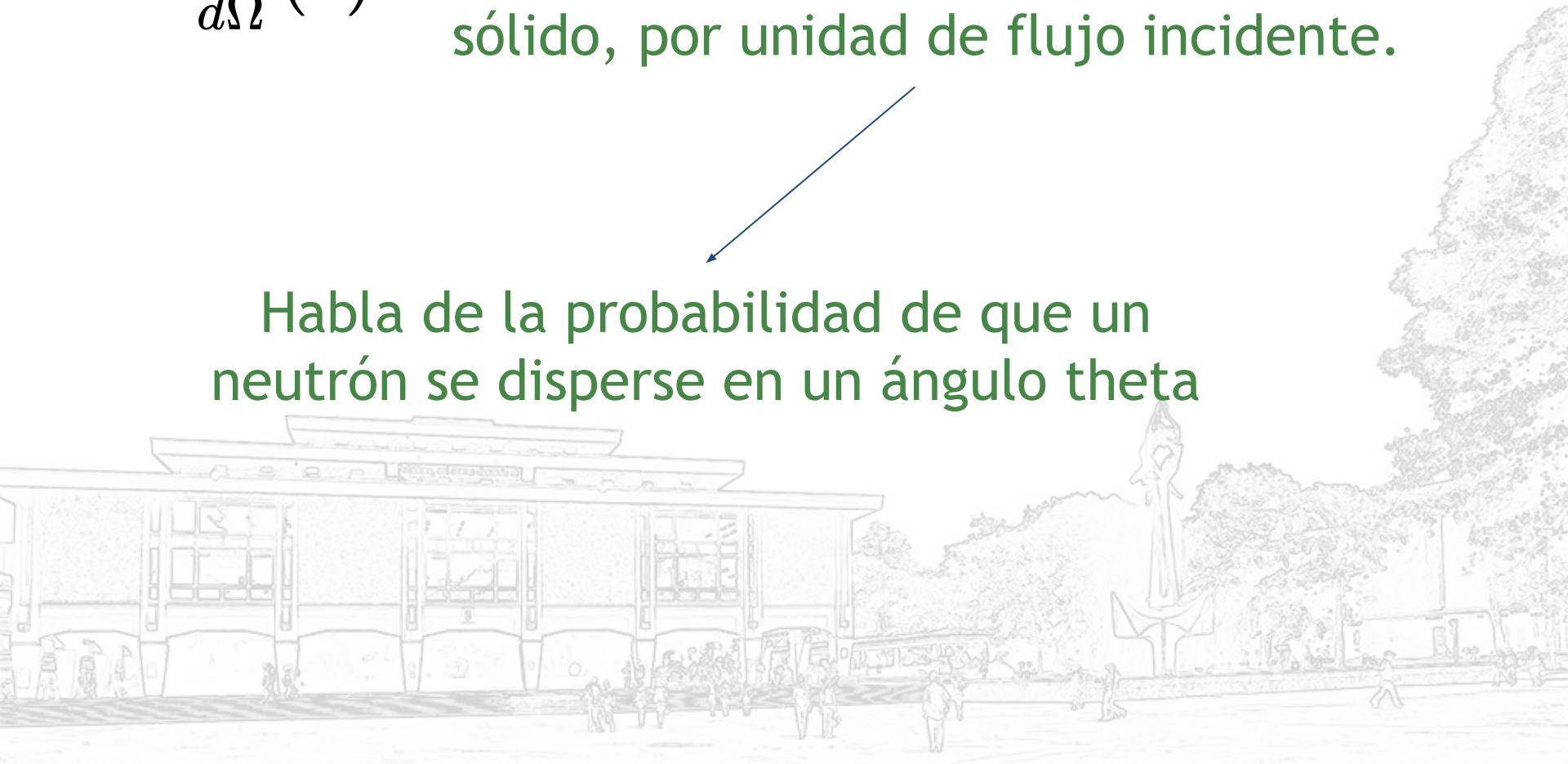
Nos interesa conocer

$$\frac{d\sigma}{d\Omega}(\theta)$$

: Flujo saliente por unidad de ángulo sólido, por unidad de flujo incidente.

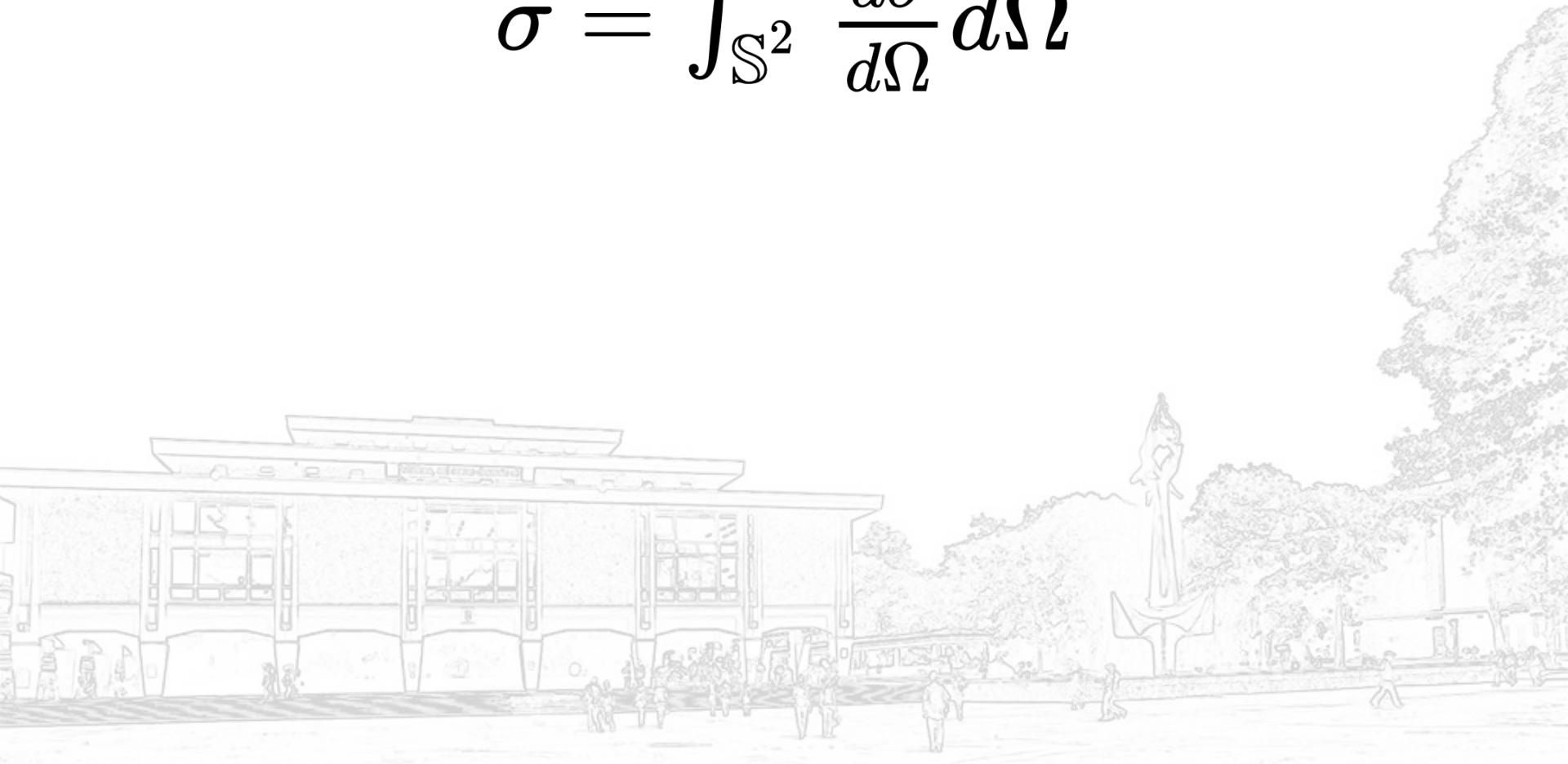


Habla de la probabilidad de que un neutrón se disperse en un ángulo theta



Adicionalmente...

$$\sigma = \int_{\mathbb{S}^2} \frac{d\sigma}{d\Omega} d\Omega$$

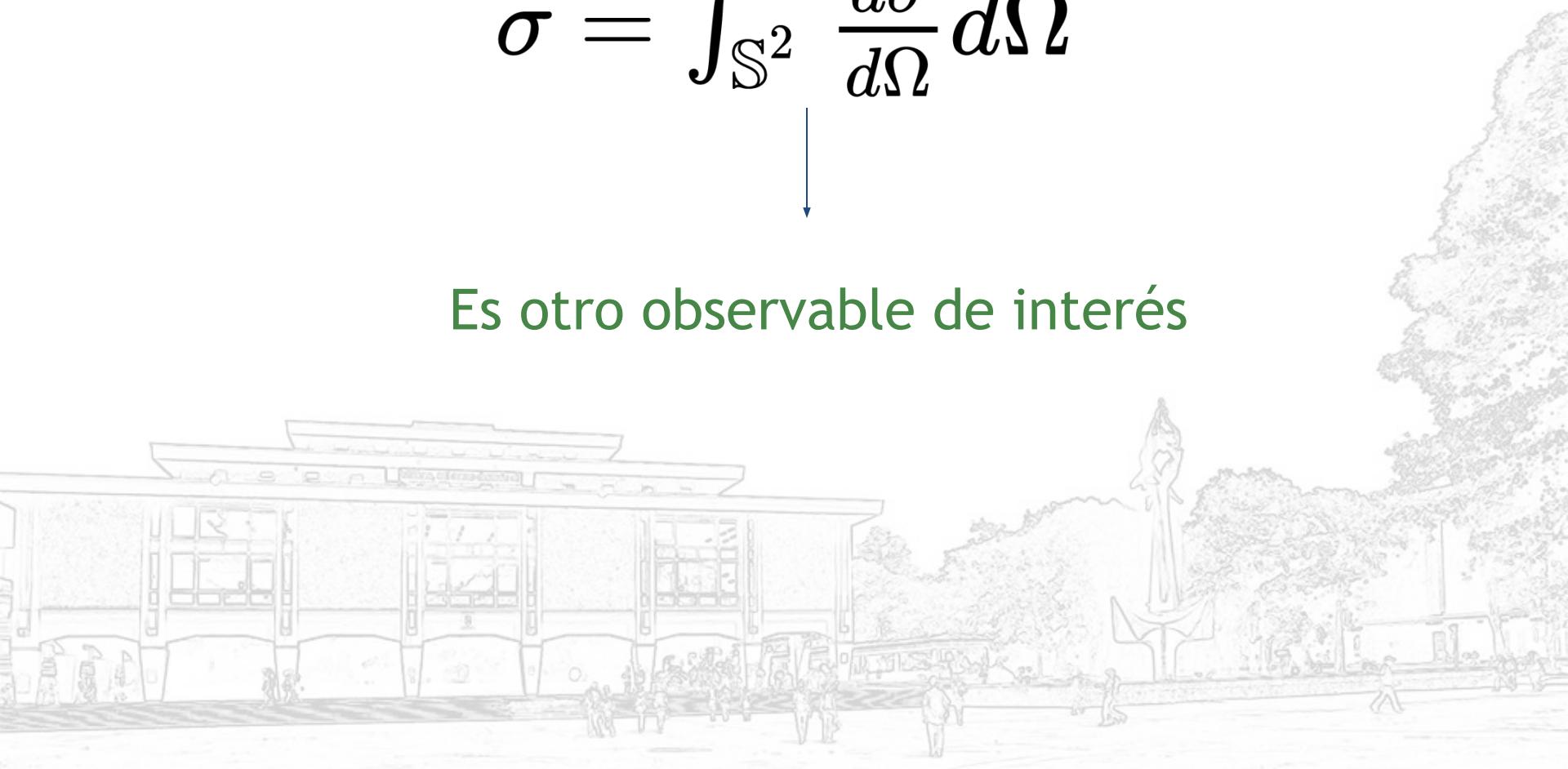


Adicionalmente,

$$\sigma = \int_{\mathbb{S}^2} \frac{d\sigma}{d\Omega} d\Omega$$



Es otro observable de interés



¿Cómo se calculan?



¿Cómo se calculan?

$$-\frac{\hbar^2}{2m} \nabla^2 \psi(\vec{r}) + V(r)\psi(\vec{r}) = E\psi(\vec{r})$$

\vec{r} : Posición relativa de las partículas al target.

$V(r)$: Potencial central que depende de la interacción entre las partículas y el target.

Condiciones de frontera



Condiciones de frontera

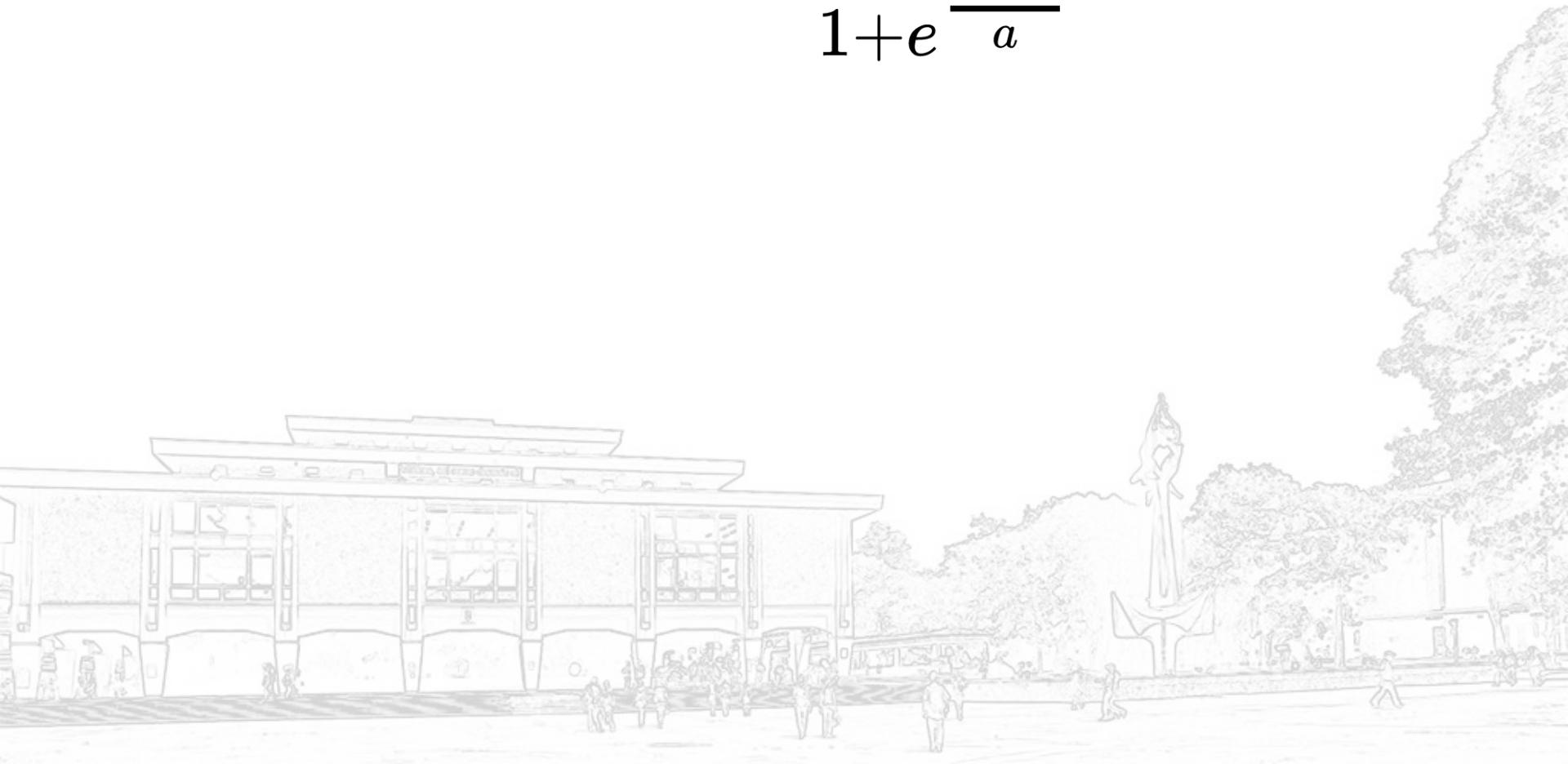
$$\psi(\vec{r}) \rightarrow_{r \rightarrow \infty} e^{ikz} + f(\theta) \frac{e^{ikr}}{r}$$

Onda plana entrante.

Onda esférica saliente.

Potencial utilizado

$$V(r) = \frac{-V_0}{1+e^{\frac{r-R}{a}}}$$



Potencial utilizado

$$V(r) = \frac{-V_0}{1 + e^{\frac{r-R}{a}}}$$

$$V_0 = V_1 - V_2 E - \left(1 - \frac{2Z}{A}\right) V_3$$

$$V_1 = 56.3 \text{ MeV} \quad V_2 = 0.32 \quad V_3 = 24.0 \text{ MeV}$$

$$R = r_0 A^{1/3} \quad r_0 = 1.17 \text{ fm} \quad a = 0.75 \text{ fm}$$

$$E \leq 50 \text{ MeV} \quad A \geq 40$$

Potencial utilizado

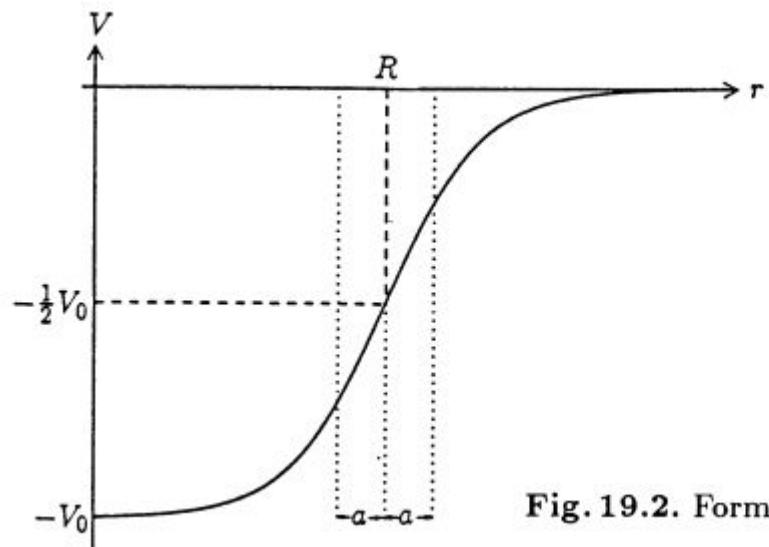


Fig. 19.2. Form of a Woods-Saxon potential

Potencial utilizado

$$b = 20\text{fm}$$

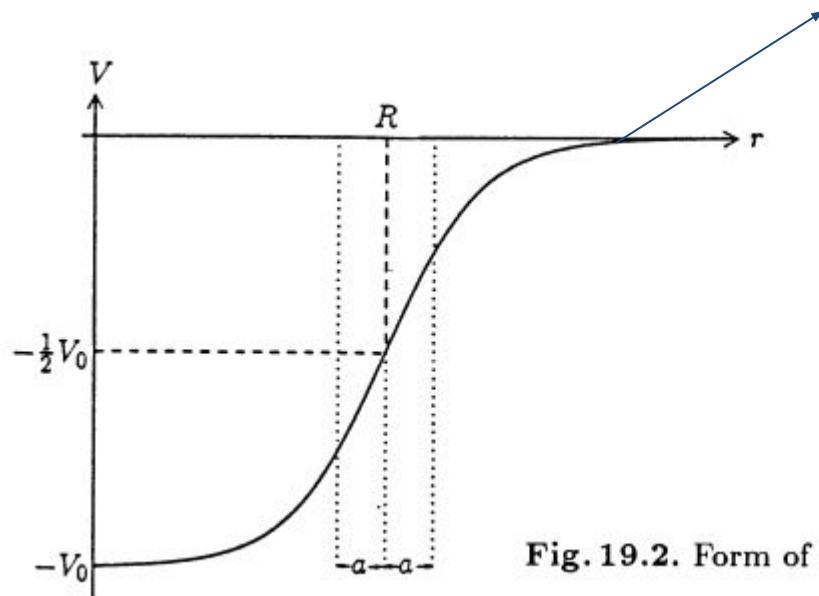


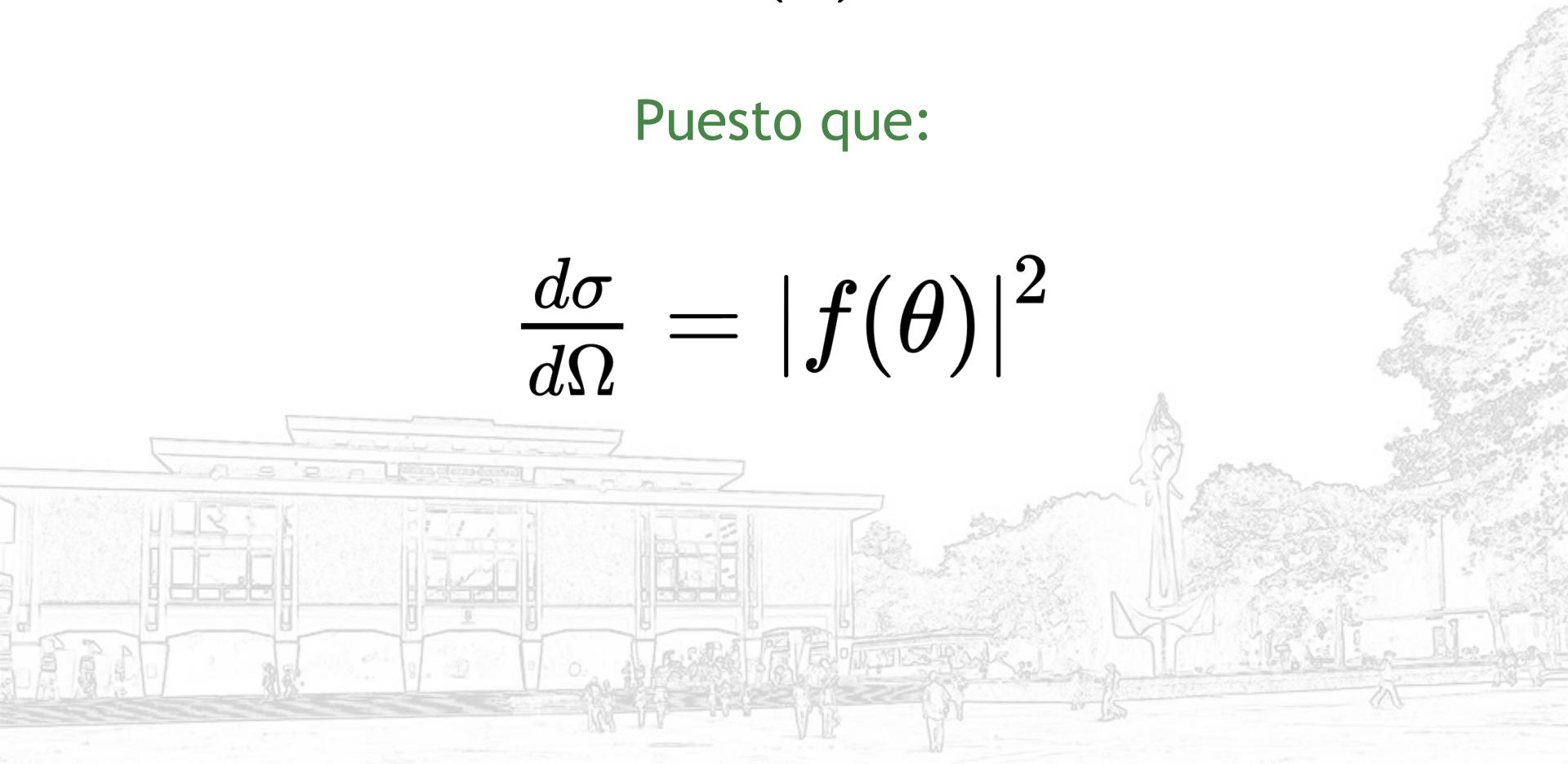
Fig. 19.2. Form of a Woods-Saxon potential

Objetivo:

$$f(\theta)$$

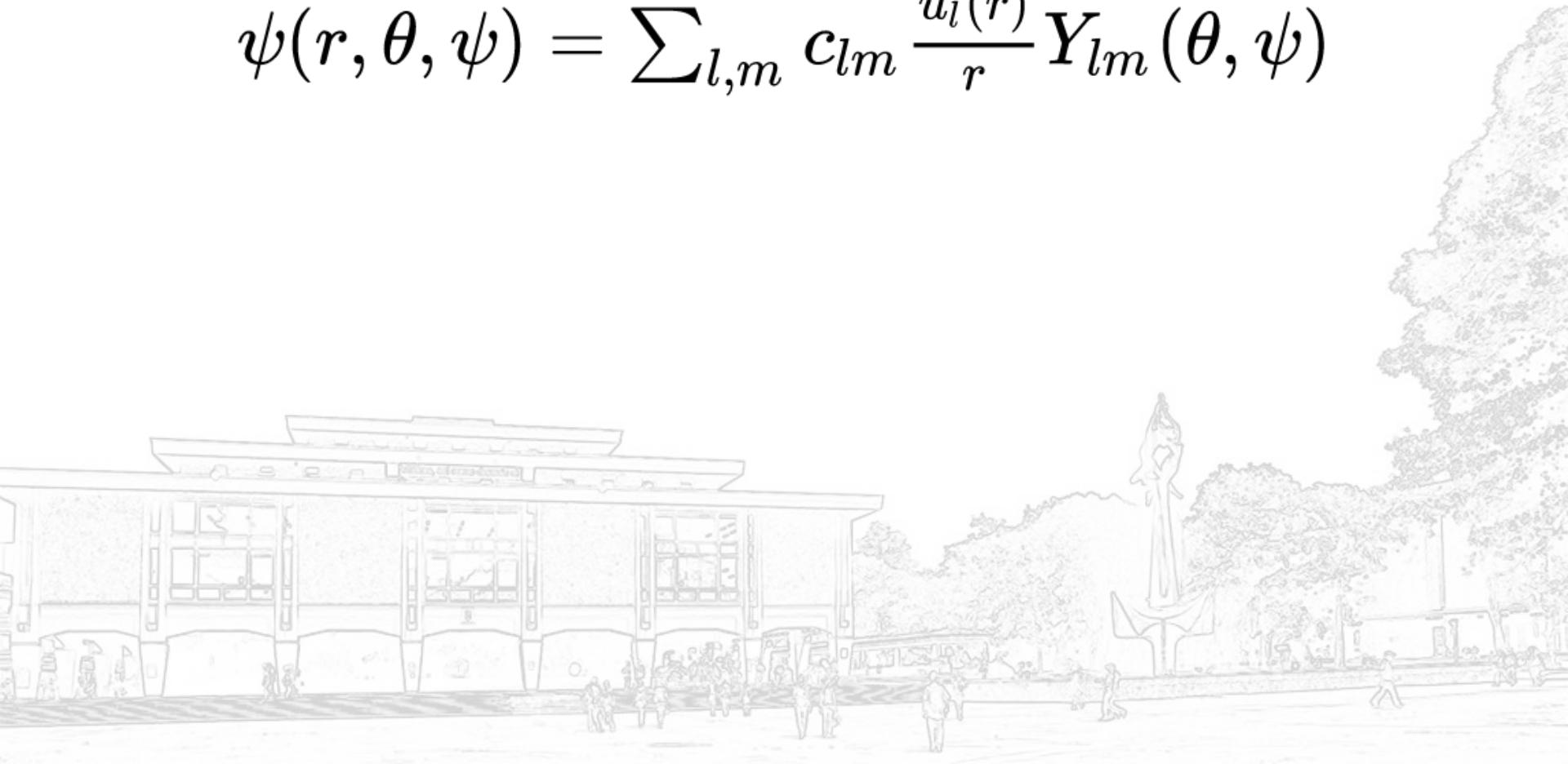
Puesto que:

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2$$



Descomposición en ondas parciales

$$\psi(r, \theta, \psi) = \sum_{l,m} c_{lm} \frac{u_l(r)}{r} Y_{lm}(\theta, \psi)$$

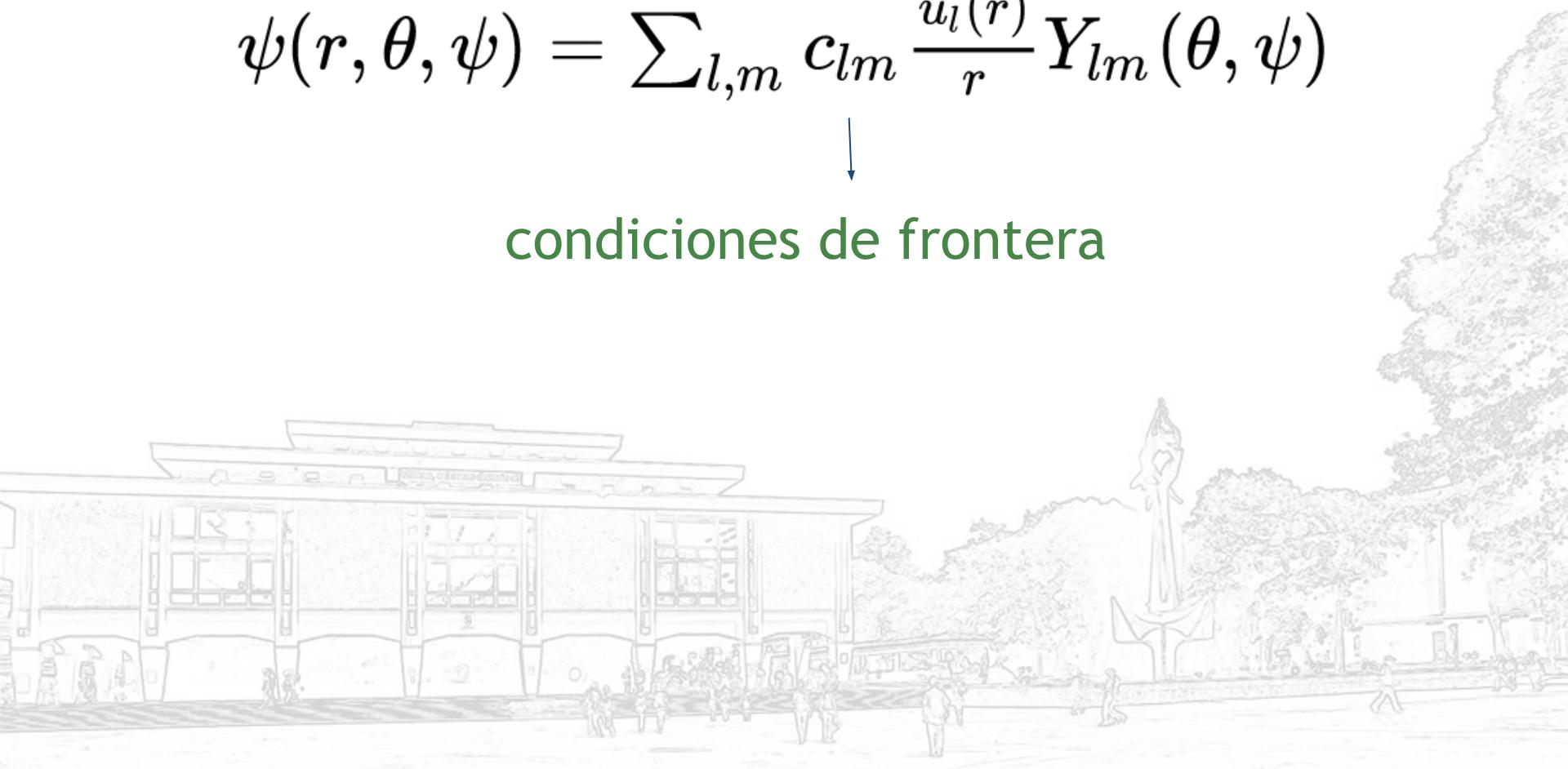


Descomposición en ondas parciales

$$\psi(r, \theta, \psi) = \sum_{l,m} c_{lm} \frac{u_l(r)}{r} Y_{lm}(\theta, \psi)$$



condiciones de frontera



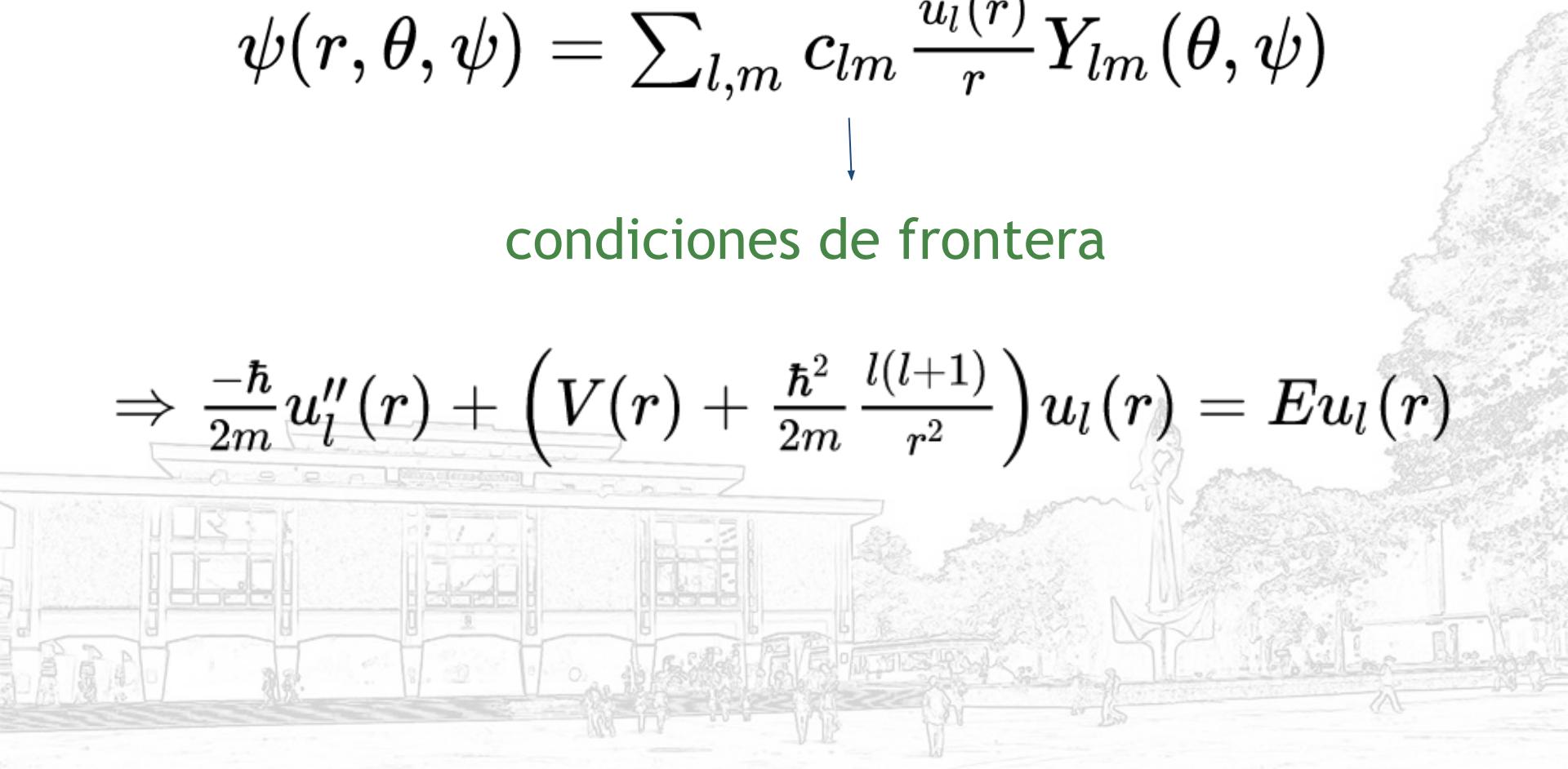
Descomposición en ondas parciales

$$\psi(r, \theta, \psi) = \sum_{l,m} c_{lm} \frac{u_l(r)}{r} Y_{lm}(\theta, \psi)$$



condiciones de frontera

$$\Rightarrow \frac{-\hbar^2}{2m} u_l''(r) + \left(V(r) + \frac{\hbar^2}{2m} \frac{l(l+1)}{r^2} \right) u_l(r) = E u_l(r)$$



Ecuación a resolver

$$\frac{-\hbar}{2m} u_l''(r) + \left(V(r) + \frac{\hbar^2}{2m} \frac{l(l+1)}{r^2} \right) u_l(r) = E u_l(r)$$

$$r \in [0, b]$$

$$\bar{u}_l''(r) + \left(k^2 - \frac{l(l+1)}{r^2} \right) \bar{u}_l(r) = 0$$

$$r > b$$

Ecuación a resolver

$$\frac{-\hbar^2}{2m} u_l''(r) + \left(V(r) + \frac{\hbar^2}{2m} \frac{l(l+1)}{r^2} \right) u_l(r) = E u_l(r)$$

$$r \in [0, b]$$

numérico

$$\bar{u}_l''(r) + \left(k^2 - \frac{l(l+1)}{r^2} \right) \bar{u}_l(r) = 0$$

$$r > b$$

¡conocido!

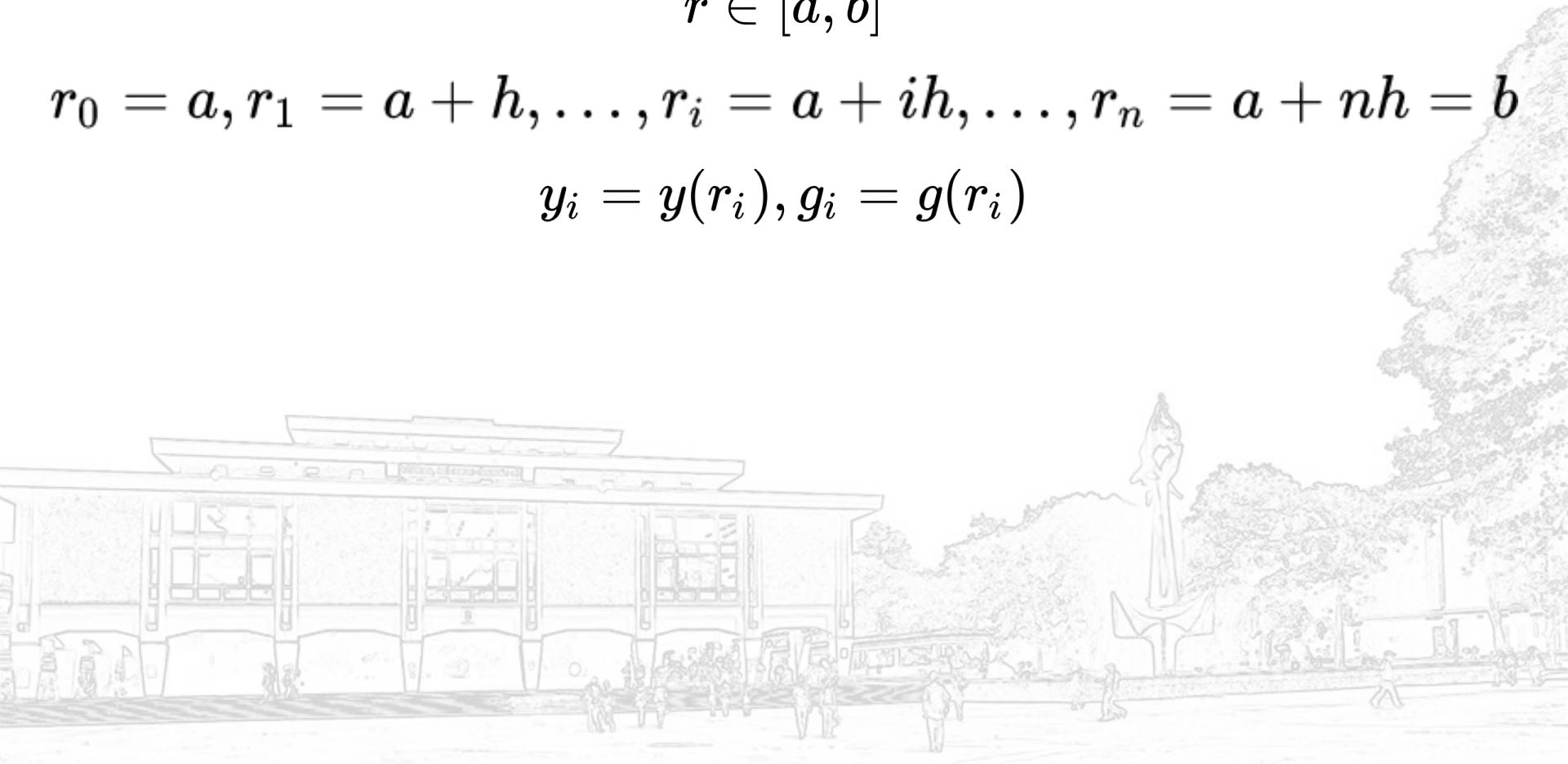
Método de Numerov

$$y''(r) + g(r)y(r) = 0$$

$$r \in [a, b]$$

$$r_0 = a, r_1 = a + h, \dots, r_i = a + ih, \dots, r_n = a + nh = b$$

$$y_i = y(r_i), g_i = g(r_i)$$



Método de Numerov

$$y''(r) + g(r)y(r) = 0$$

$$r \in [a, b]$$

$$r_0 = a, r_1 = a + h, \dots, r_i = a + ih, \dots, r_n = a + nh = b$$

$$y_i = y(r_i), g_i = g(r_i)$$

$$y_{i+1} = y_i + y'_i h + \frac{y''_i}{2!} h^2 + \frac{y^{(3)}_i}{3!} h^3 + \frac{y^{(4)}_i}{4!} h^4 + \frac{y^{(5)}_i}{5!} h^5 + O(6)$$

$$y_{i-1} = y_i - y'_i h + \frac{y''_i}{2!} h^2 - \frac{y^{(3)}_i}{3!} h^3 + \frac{y^{(4)}_i}{4!} h^4 - \frac{y^{(5)}_i}{5!} h^5 + O(6)$$

Método de Numerov

$$y_{i+1} - 2y_i + y_{i-1} = h^2 y''_i + \frac{h^4}{12} y_i^{(4)} + O(h^6)$$

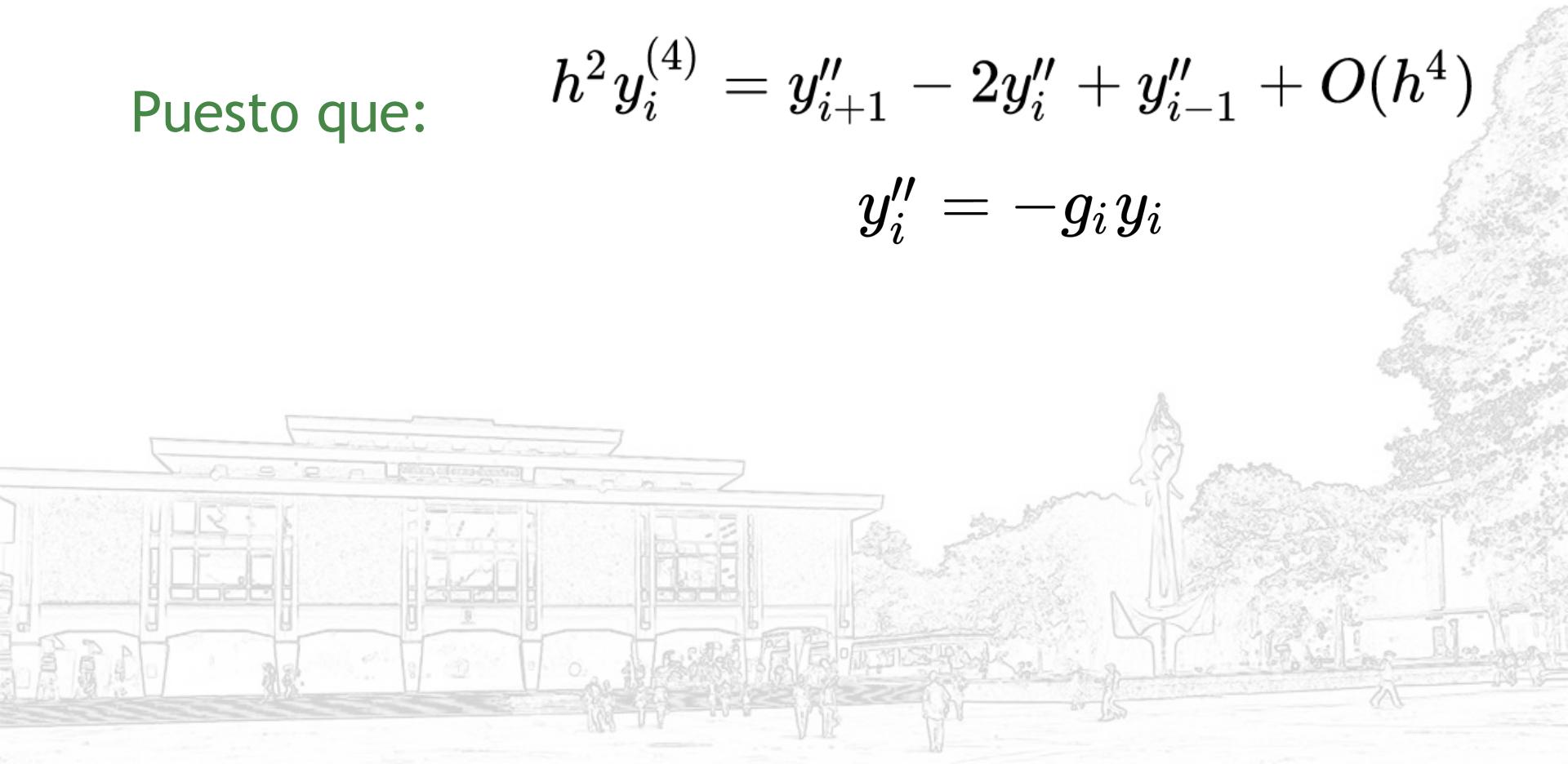


Método de Numerov

$$y_{i+1} - 2y_i + y_{i-1} = h^2 y''_i + \frac{h^4}{12} y^{(4)}_i + O(h^6)$$

Puesto que: $h^2 y^{(4)}_i = y''_{i+1} - 2y''_i + y''_{i-1} + O(h^4)$

$$y''_i = -g_i y_i$$



Método de Numerov

$$y_{i+1} - 2y_i + y_{i-1} = h^2 y''_i + \frac{h^4}{12} y^{(4)}_i + O(h^6)$$

Puesto que: $h^2 y^{(4)}_i = y''_{i+1} - 2y''_i + y''_{i-1} + O(h^4)$

$$y''_i = -g_i y_i$$

Se obtiene después de un
poco de álgebra:

$$y_{i+1} = \frac{2y_i \left(1 - \frac{5h^2}{12} g_i\right) - y_{i-1} \left(1 + \frac{h^2}{12} g_{i-1}\right)}{1 + \frac{h^2}{12} g_{i+1}}$$

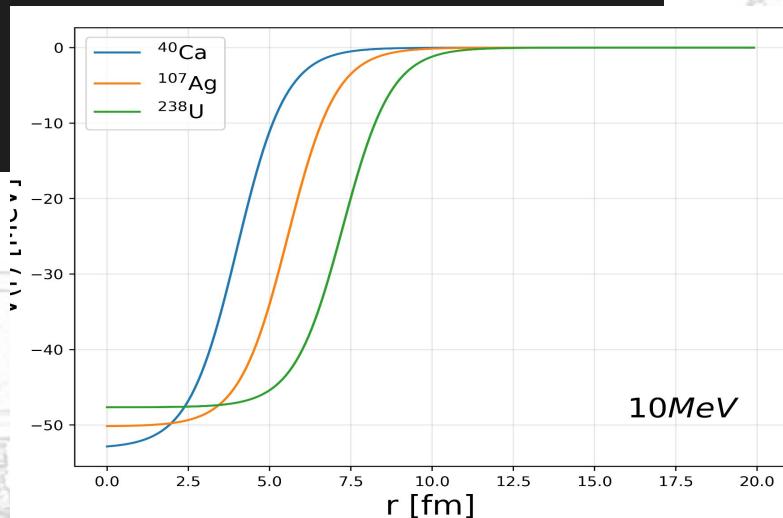
Simulaciones

- Potencial

```
// Función para calcular el potencial de Wood-Saxon
void WoodSaxon::Potencial(){

    double V1 = 56.3, V2 = 0.32, V3 = 24.0;          // Constantes del potencial en [MeV]
    double a = 0.75, r0 = 1.17, expmax = 700;        // Constantes del potencial en [fm]
    double R = r0*pow(A, 1.0/3.0);                  // Radio del núcleo
    double V0= V1-V2*E-V3*(1.0-(2.0*Z)/A);        // Profundidad del pozo del potencial

    for (int i = 0; i < N; i++){
        if ((r[i]-R)/a <= expmax){
            V.push_back(-V0/(1.0 + exp((r[i]-R)/a)));
        }
        else{
            V.push_back(0.0);
        }
    }
}
```



Simulaciones

- Método de Numerov

```
W0=(E-V[0])/H2M-l*(l+1)/(dx*dx);           // Valor de g(0) de acuerdo a su definición
W1=(E-V[1])/H2M-l*(l+1)/(dx*dx);           // Valor de g(h) de acuerdo a su definición
U0=0.0;                                      // Se inicializa f(0) = 0 para garantizar la continuidad de R(r)
U1=1.0;                                      // Se inicializa f(h) = 1

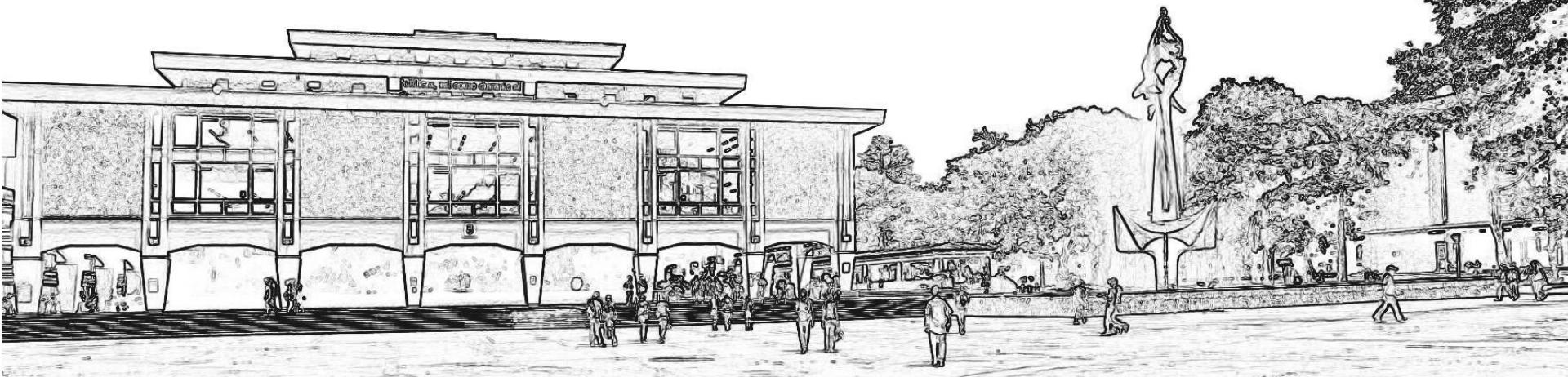
for(int i=1; i<N-1;i++){                     // Método de Numerov

    R=r[i+1];
    W2= (E-V[i+1])/H2M-l*(l+1)/(R*R);
    U2=((2*U1)-U0-(( (dx*dx)/12.0)*((10*W1*U1)+(W0*U0)) ))/(1+dx*dx*W2/12);
    W0=W1;
    W1=W2;
    U0=U1;
    U1=U2;
}
```

$$W_i = g(r = idx) = \frac{2m}{\hbar^2} (E - V(r)) - \frac{l(l+1)}{r^2}$$



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Obtención de la sección
eficaz

Si el potencial decae a cero aproximadamente
a distancia b

$$\bar{u}_l(r) = a_l kr [\cos(\delta_l) j_l(kr) - \sin(\delta_l) \eta_l(kr)]$$

$$r > b$$

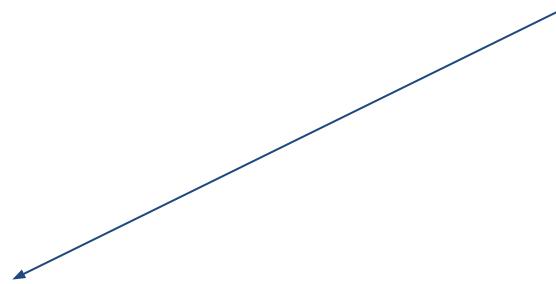
$$\tan(\delta_l) = \frac{(b-h)j_l(k(b-h))u_l(b)-bj_l(kb)u_l(b-h)}{(b-h)\eta_l(k(b-h))u_l(b)-b\eta_l(kb)u_l(b-h)}$$

u_l

Solución numérica en la región donde el
potencial es efectivo, con los parámetros
definidos anteriormente

Amplitud angular:

$$f(\theta) = \frac{1}{k} \sum_{l \geq 0} (2l + 1) e^{i\delta_l} \sin(\delta_l) P_l(\cos(\theta))$$



Polinomios de Legendre

Sección eficaz

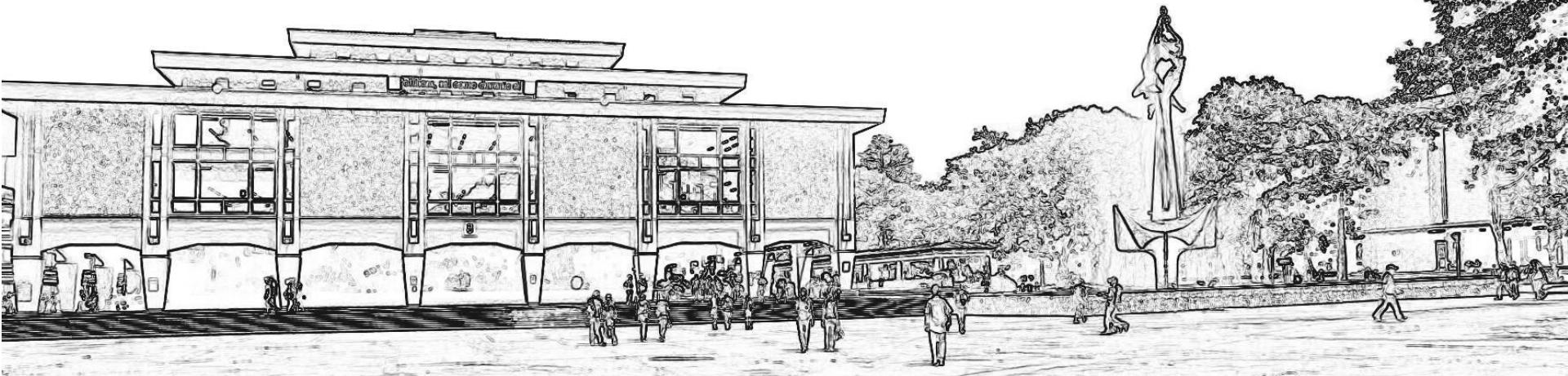
$$\frac{d\sigma}{d\Omega}(\theta) = \frac{1}{k^2} \left| \sum_{l=0} (2l+1) e^{i\delta_l} \sin(\delta_l) P_l(\cos(\theta)) \right|^2$$

$$\sigma = \frac{4\pi}{k^2} \sum_{l \geq 0} (2l+1) \sin^2(\delta_l)$$





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Algoritmos y simulación

Simulaciones

- Sección eficaz diferencial y total

```
// Cálculo de la sección eficaz diferencial
void WoodSaxon::SeccionEficazDif(){
    // deg: Factor de conversión de radianes a grados
    // Ref: Parte real de la amplitud de dispersión
    // Imf: Parte imaginaria de la amplitud de dispersión
    // plth: Polinomio de Legendre evaluado en cos θ

    double deg= M_PI/180,Ref,Imf,plth;
    dsigma.clear();
    for(int i=0; i<=180; i++){
        theta.push_back(i*deg);
        Ref=0.0;
        Imf=0.0;
        for(int l=0;l<lp_conv+1;l++){           // Cálculo de la parte real e imaginaria
            plth = legendre(l,cos(theta[i]));
            Ref = Ref+ (0.5/k)*(2*l+1)*(sin(2*delta[l]))*plth;
            Imf = Imf+(l/k)*(2*l+1)*(pow(sin(delta[l]),2))*plth;
        }
        dsigma.push_back(Ref*Ref+Imf*Imf);      // Se calcula dσ/dΩ = Re(f(θ))**2 + Im(f(θ))**2 para el θ del ciclo
        if (i==0){
            sigma = (4*M_PI/k)*Imf*10;          // Se calcula la sección eficaz total σ = 4πh(0)/k
        }
    }
}
```

$$g(\theta) := \frac{1}{2k} \sum_{l=0}^{\infty} (2l + 1) \sin(2\delta_l) P_l(\cos \theta)$$

$$h(\theta) := \frac{1}{k} \sum_{l=0}^{\infty} (2l + 1) \sin^2(\delta_l) P_l(\cos \theta)$$

$$\frac{d\sigma}{d\Omega} = (g(\theta))^2 + (h(\theta))^2,$$

$$\sigma = \frac{4\pi}{k} h(0).$$

Estructura del código

```
class WoodSaxon{

public:
    WoodSaxon(double, double, unsigned int , unsigned int, string);
    void Calcular();
    void Potencial();
    void NumerovMethod(unsigned int);
    void SigmaConv();
    void SeccionEficazDif();
    void Guardar(string, int);
    double sigma;

private:
    double Rmax=20.0, dx=0.1;
    double E, H2M, k, Mass;
    int N;
    unsigned int A, Z, lp_conv;
    vector <double> r;
    vector <double> V;
    vector <double> delta;
    vector <double> theta, dsigma, LP, sigmarrayConv;
    string Elem;
};

class Resonancias{

public:
    Resonancias(double, unsigned int , unsigned int, string);
};

#endif
```



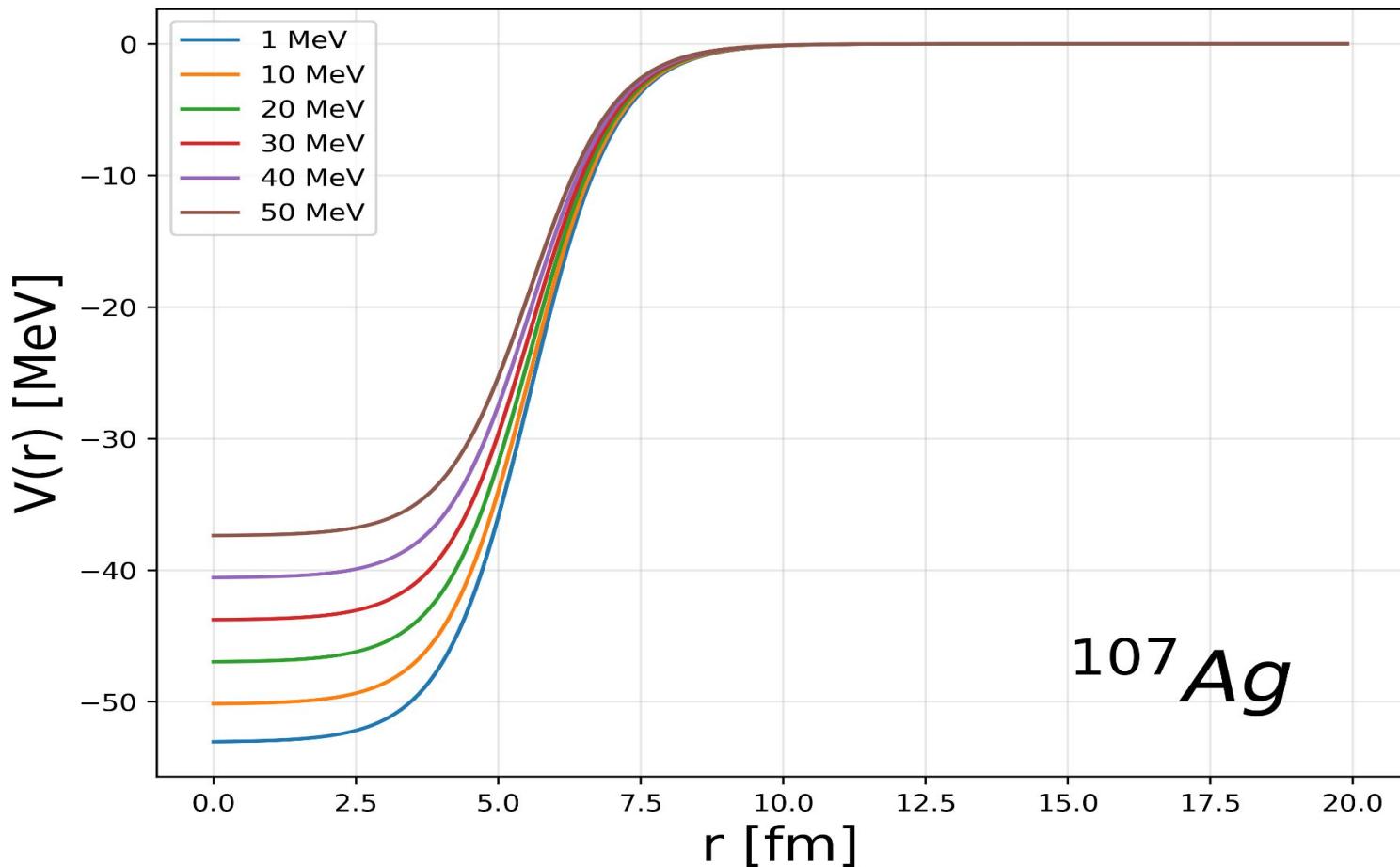
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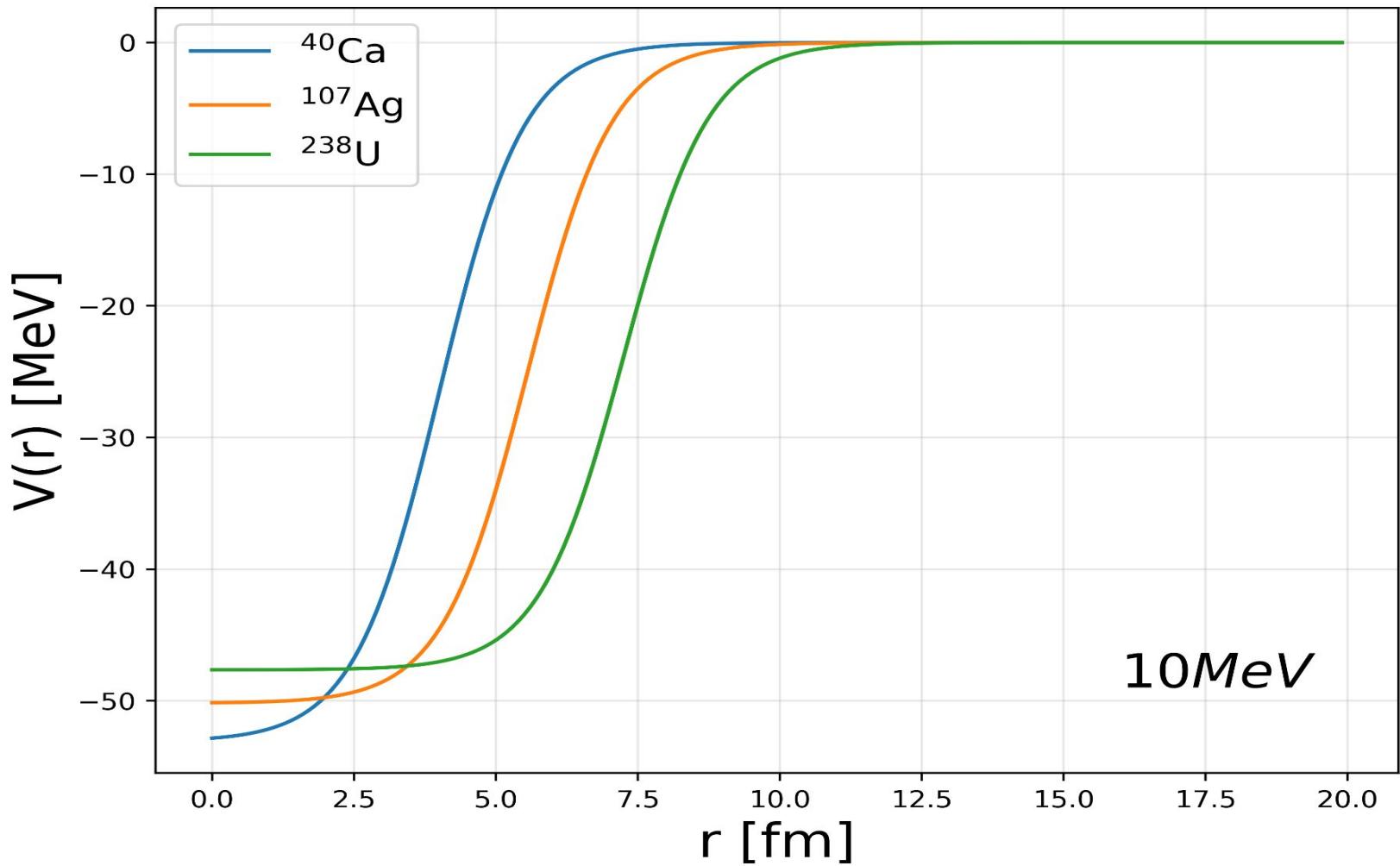
Resultados y análisis con
medidas

Potenciales

$$V(r) = \frac{-V_0}{1+e^{\frac{r-R}{a}}} \quad V_0 = V_1 - V_2 E - \left(1 - \frac{2Z}{A}\right) V_3$$

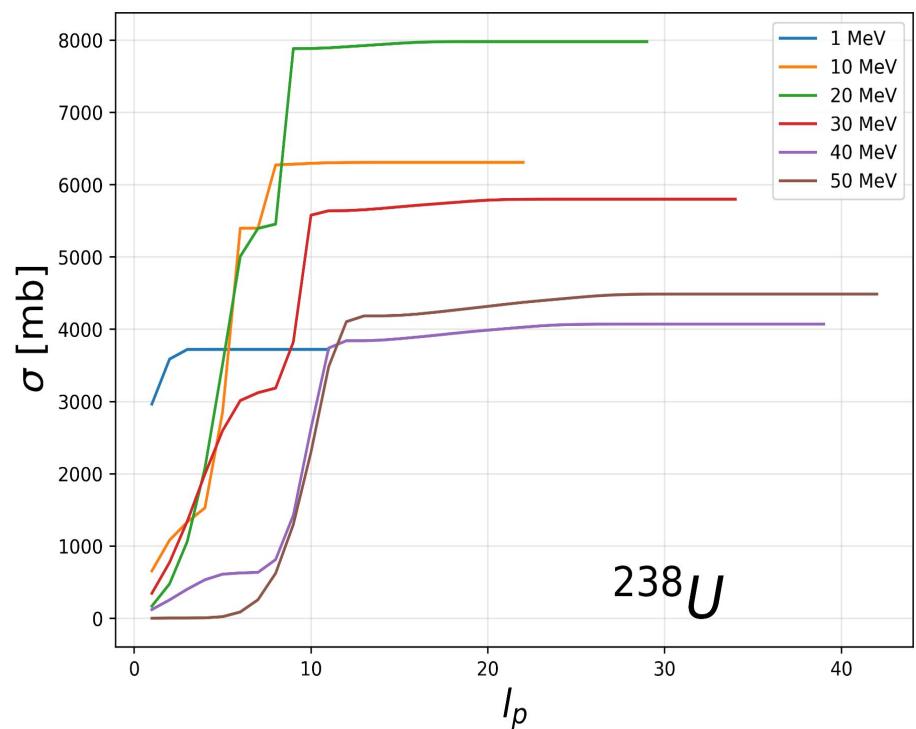
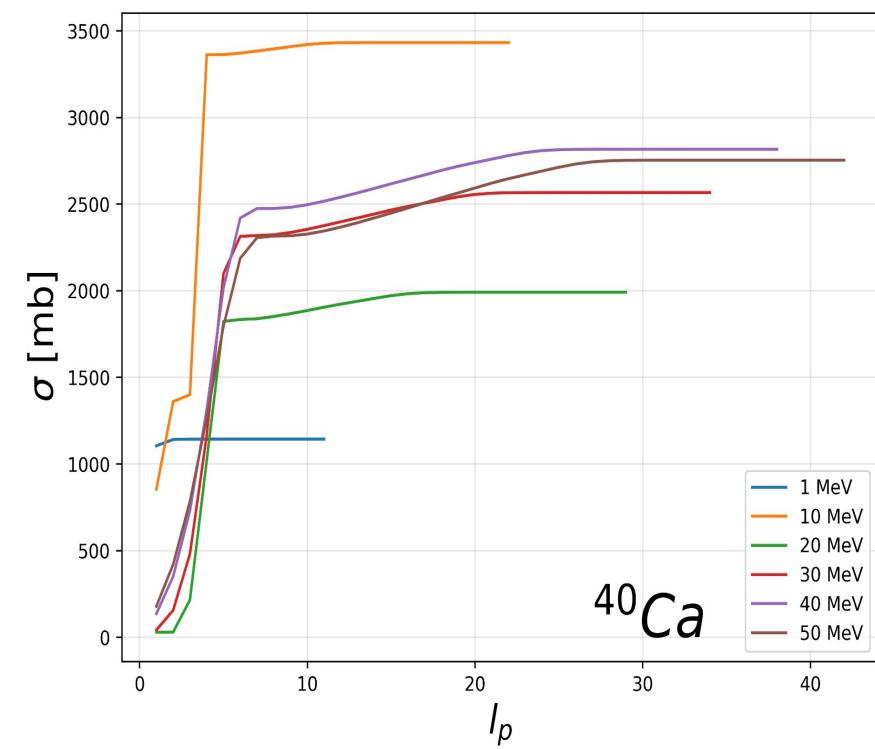


$$R = r_0 A^{1/3}$$



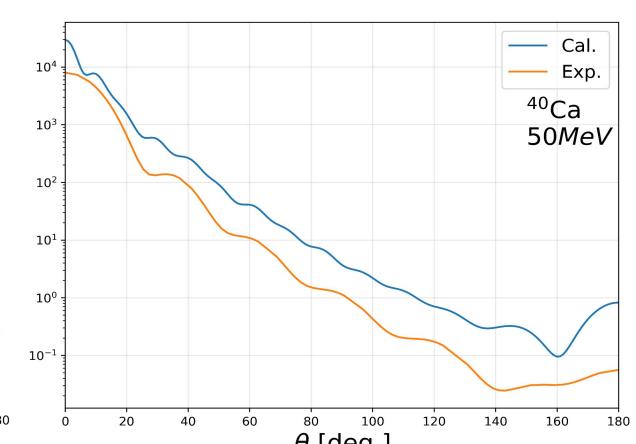
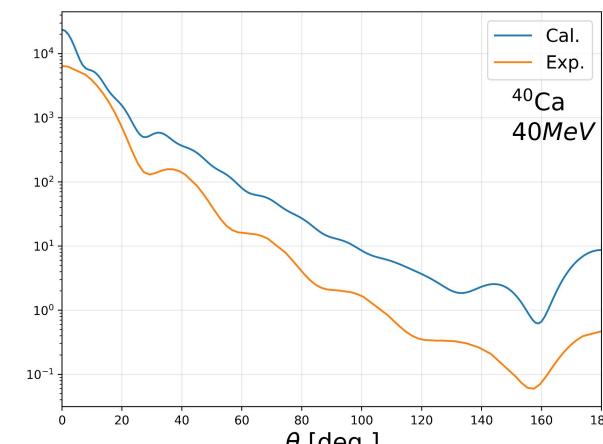
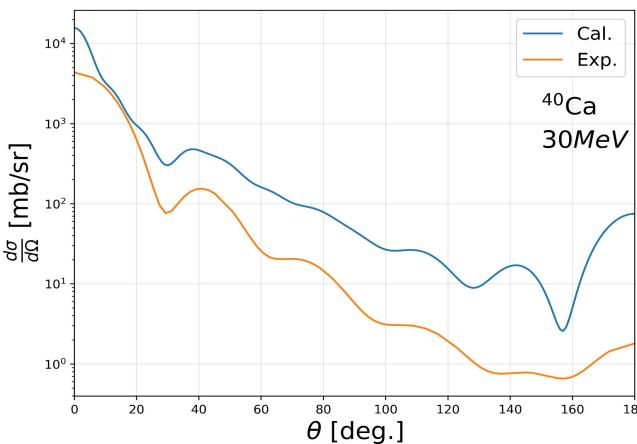
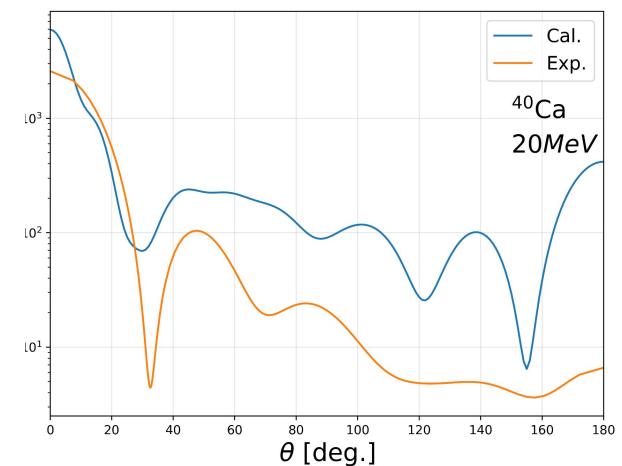
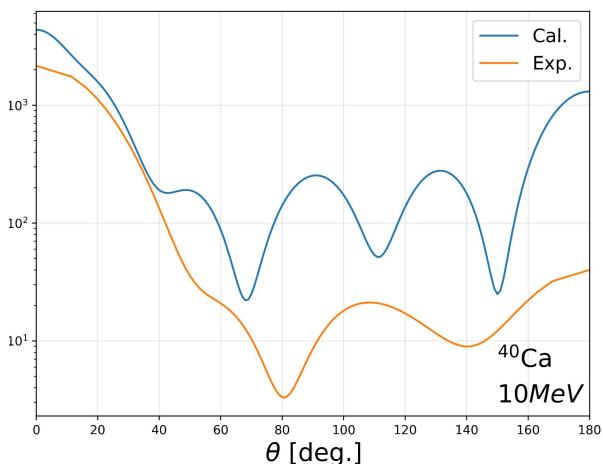
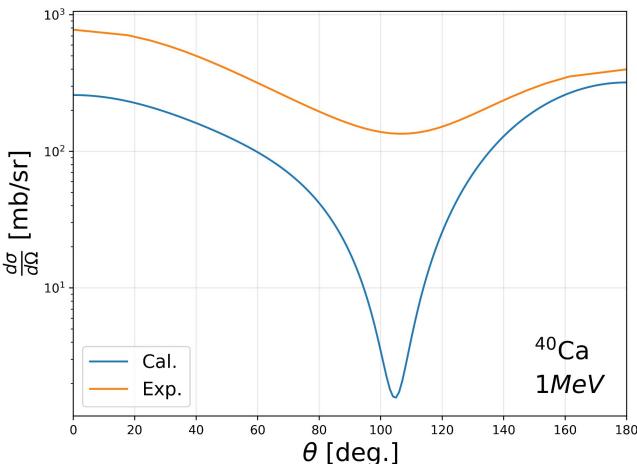
l de convergencia

$$\psi(r, \theta, \psi) = \sum_{l,m} c_{lm} \frac{u_l(r)}{r} Y_{lm}(\theta, \psi)$$



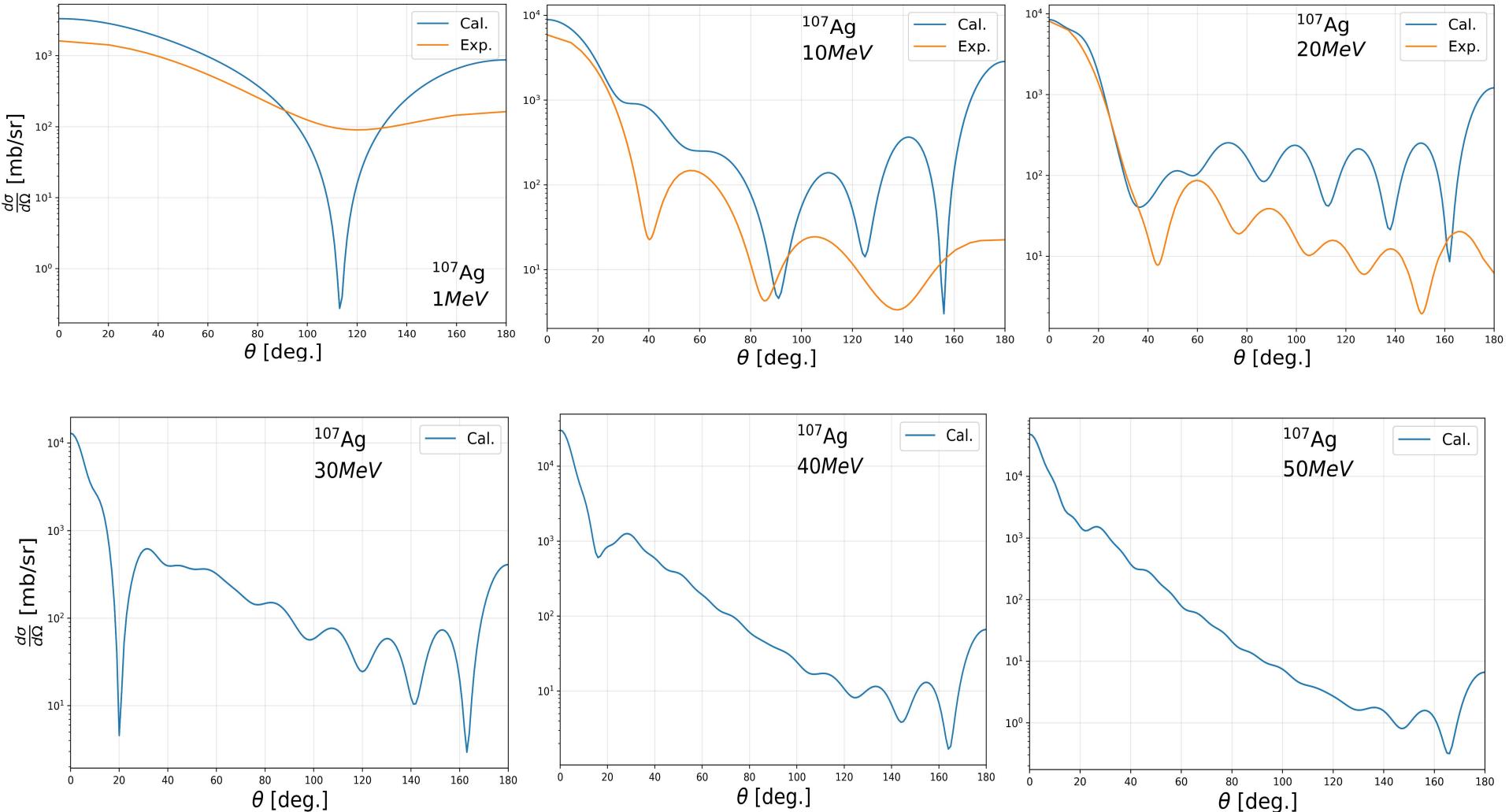
Secciones Eficaces diferenciales

10 -



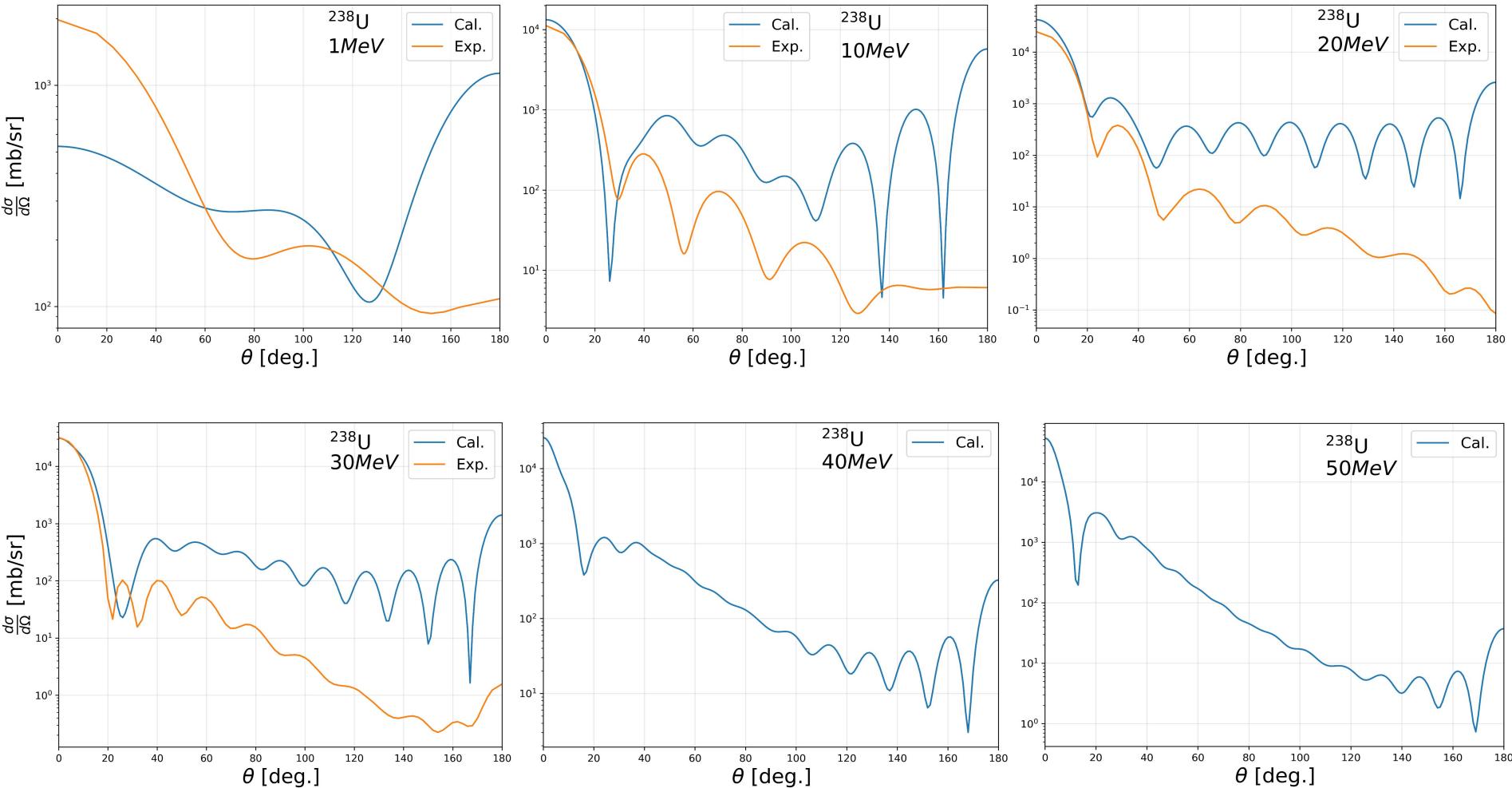
Secciones Eficaces diferenciales

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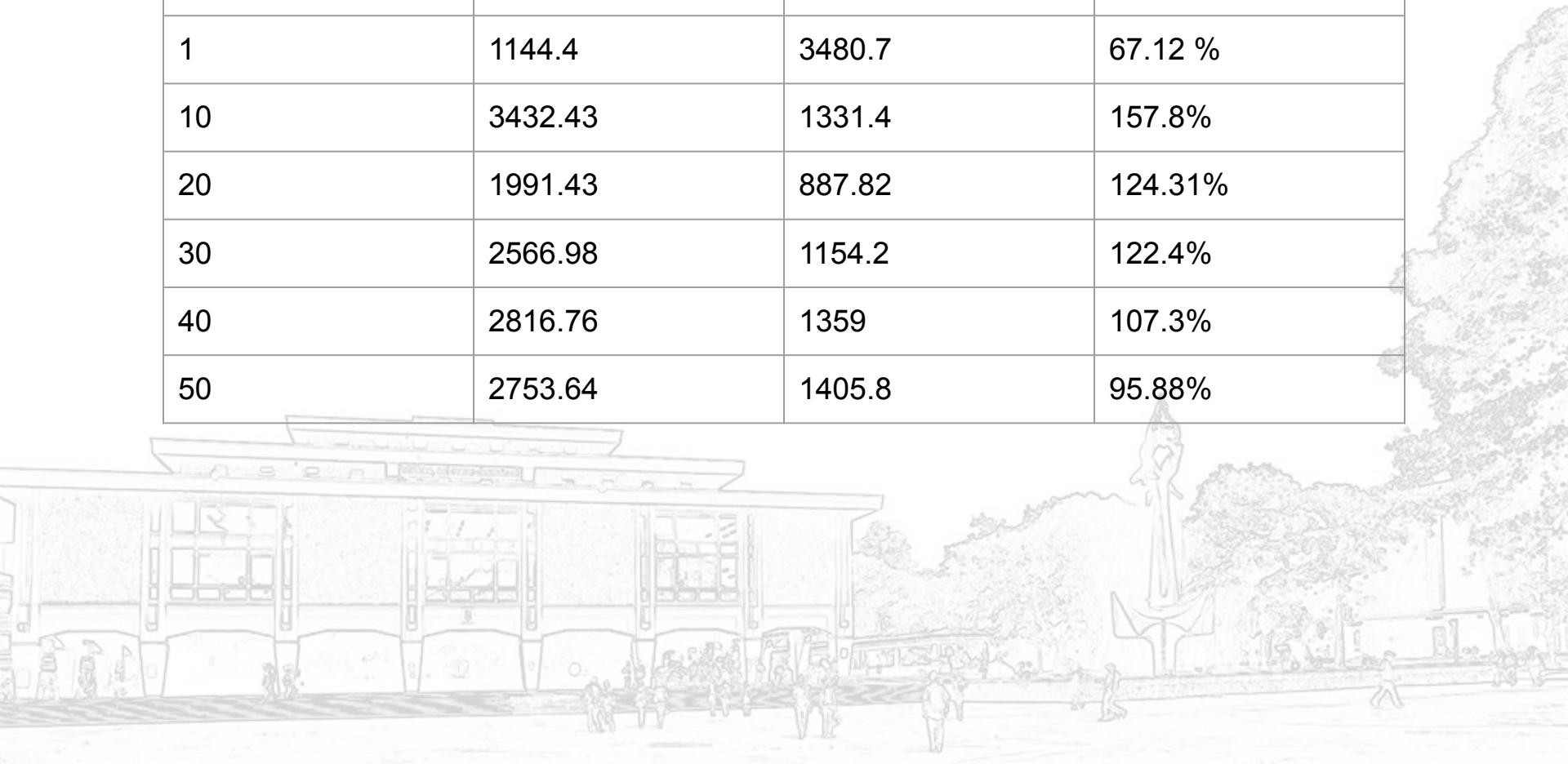
Secciones Eficaces diferenciales

228..



Calcio

Energy(Mev)	σ Simulado	σ Experimental	Error relativo
1	1144.4	3480.7	67.12 %
10	3432.43	1331.4	157.8%
20	1991.43	887.82	124.31%
30	2566.98	1154.2	122.4%
40	2816.76	1359	107.3%
50	2753.64	1405.8	95.88%

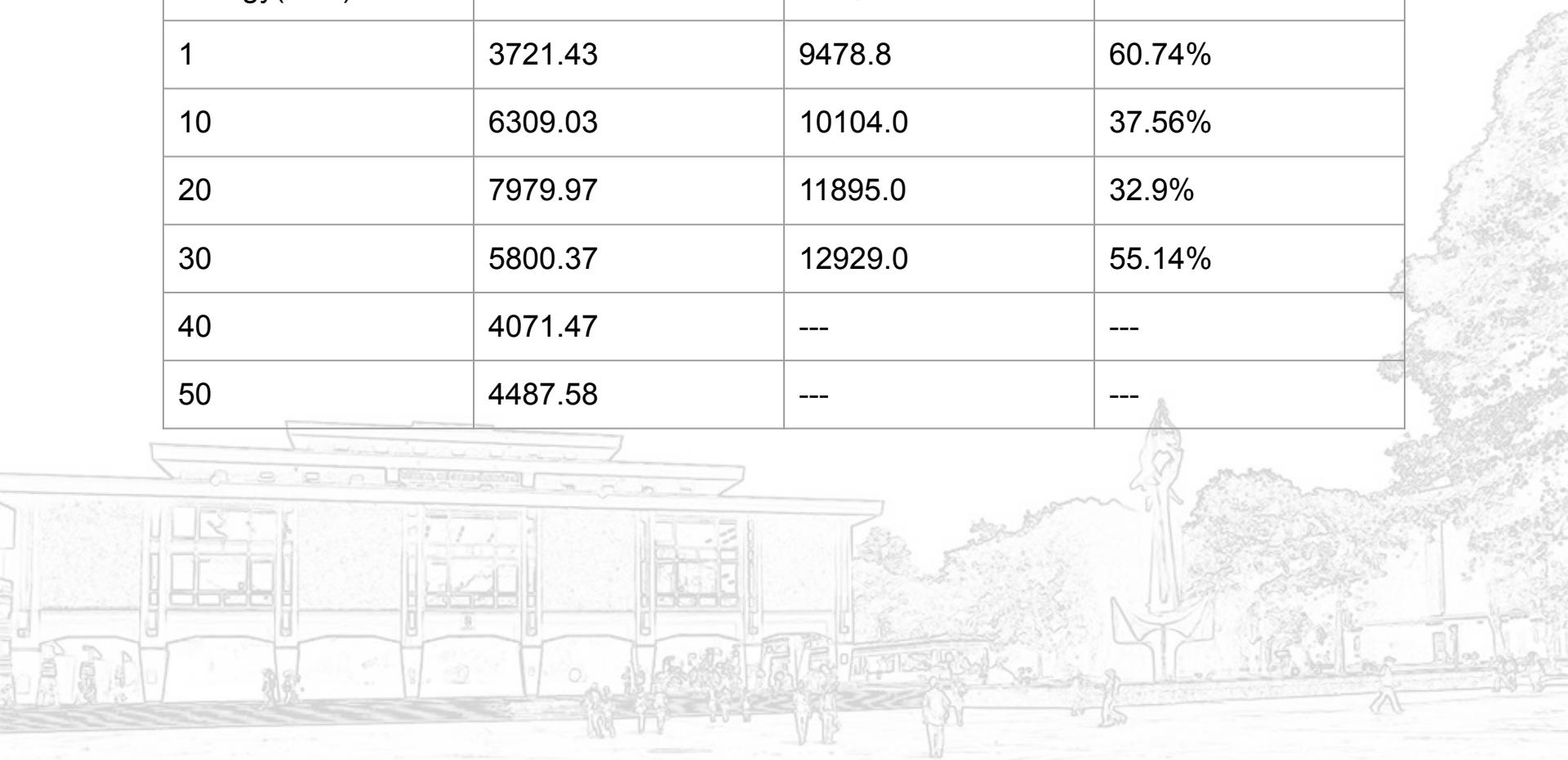


Plata

Energy(Mev)	σ Simulado	σ Experimental	Error relativo
1	8699.29	4912.55	77.08 %
10	5404.94	2432.2	122.22 %
20	3698.92	2036.5	81.63%
30	2758.15	---	---
40	3343.53	---	---
50	4038.3	---	---

Uranio

Energy(Mev)	σ Simulado	σ Experimental	Error relativo
1	3721.43	9478.8	60.74%
10	6309.03	10104.0	37.56%
20	7979.97	11895.0	32.9%
30	5800.37	12929.0	55.14%
40	4071.47	---	---
50	4487.58	---	---

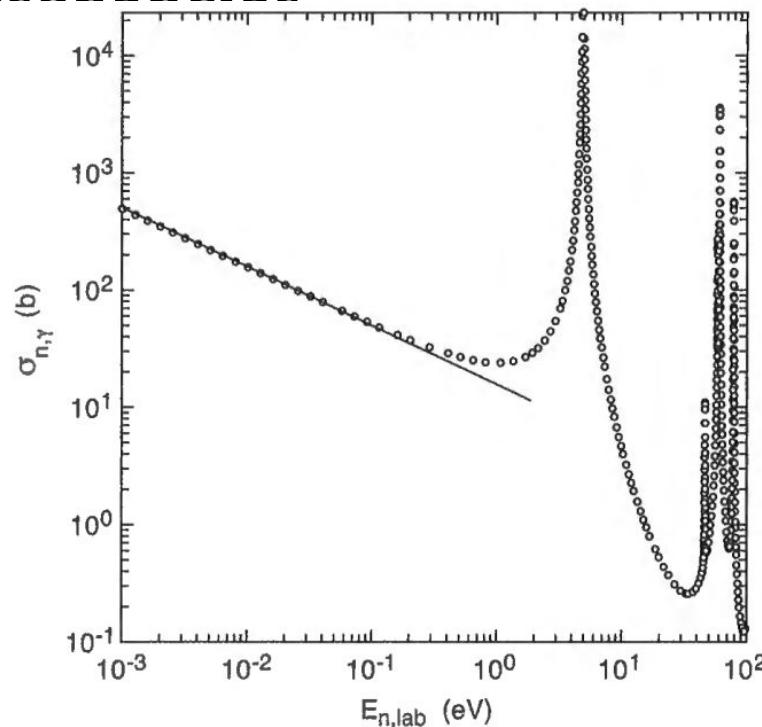


Resonancias

A bajas energías la sección transversal sigue una forma como

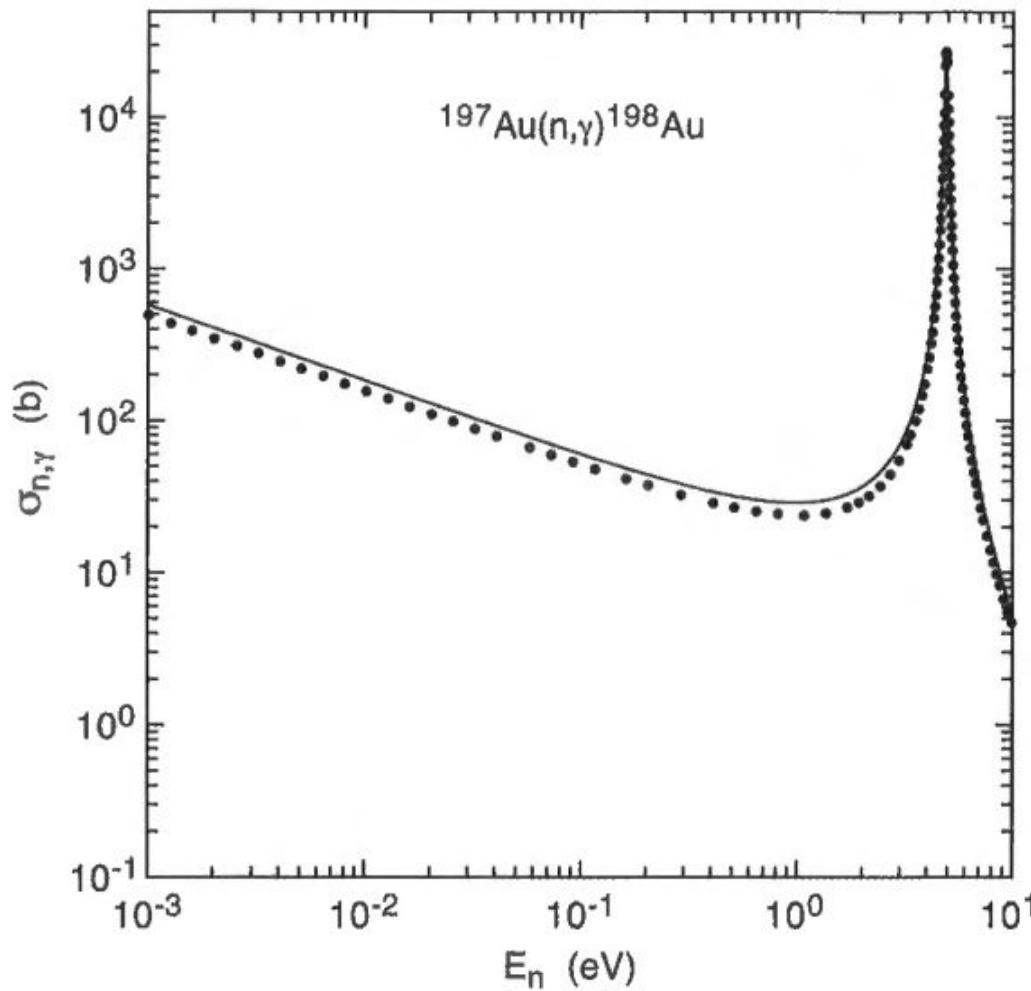
$$\sigma(E) \propto 1/\sqrt{E}$$

Las desviaciones de esta forma funcional se denominan ~~resonancias~~

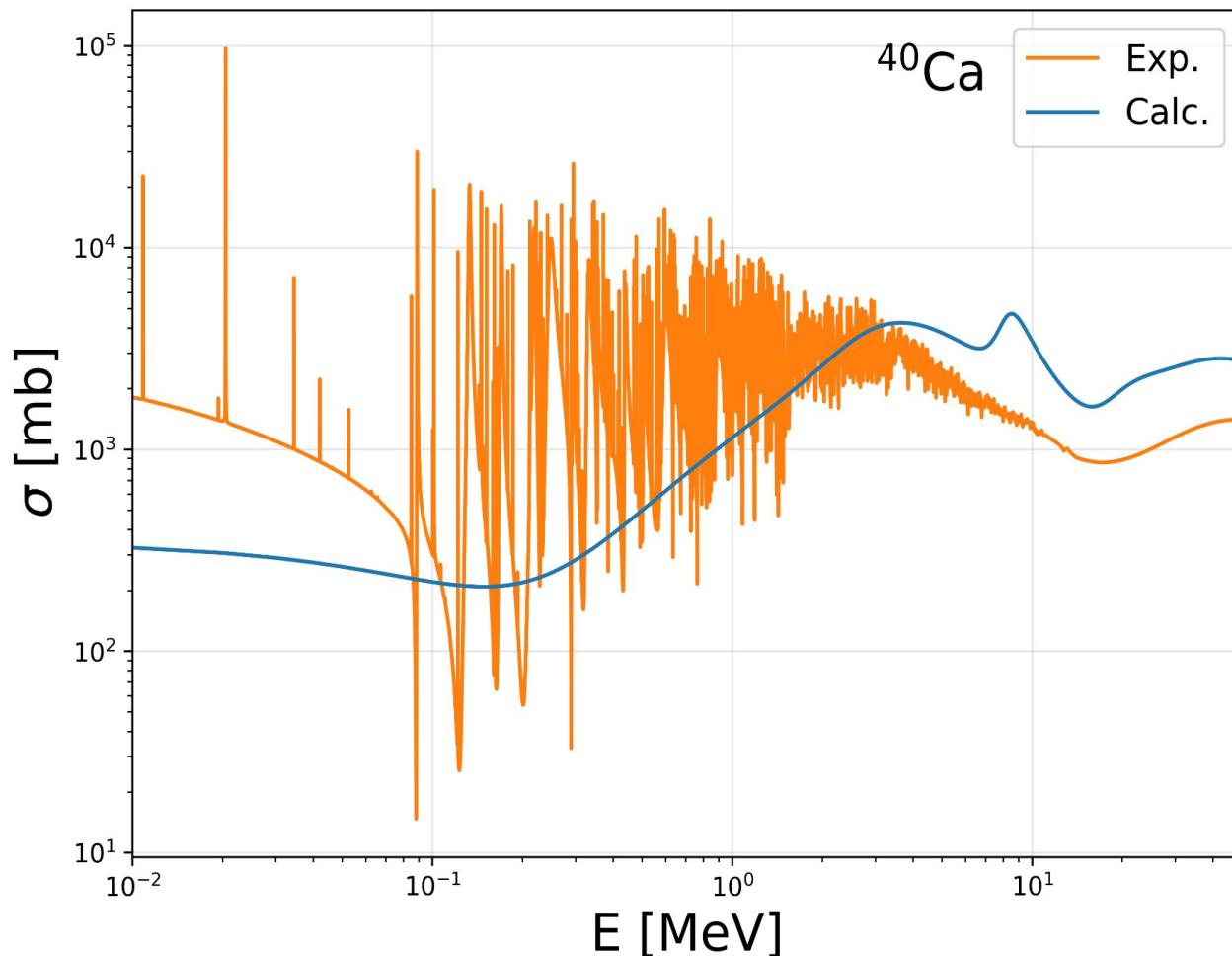


Distribución de Breit-Wigner:

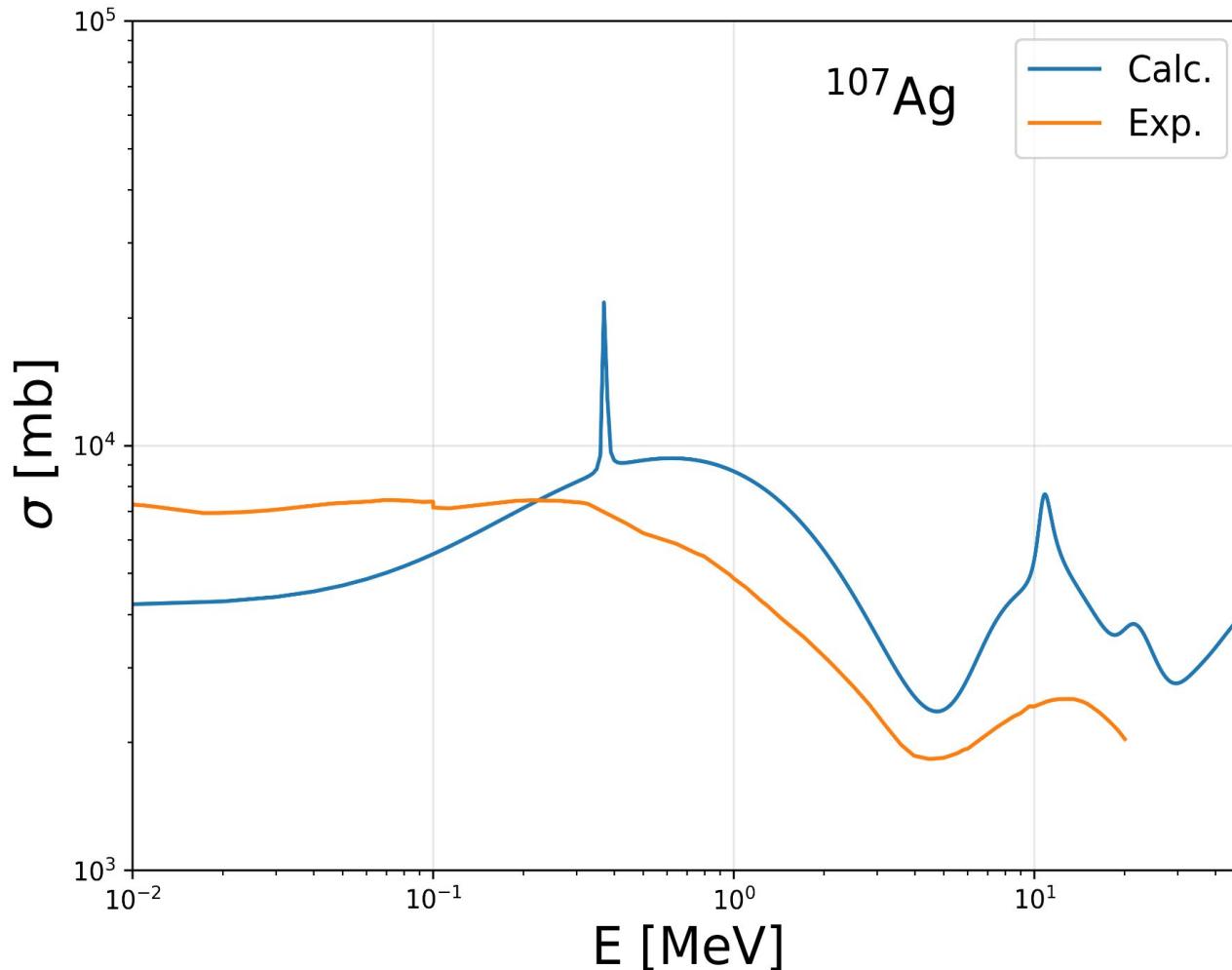
$$\sigma_{a,b}(E) = \pi g \lambda_a^2 \frac{\Gamma_a \Gamma_b}{(E - E_0)^2 + \Gamma^2/4}$$



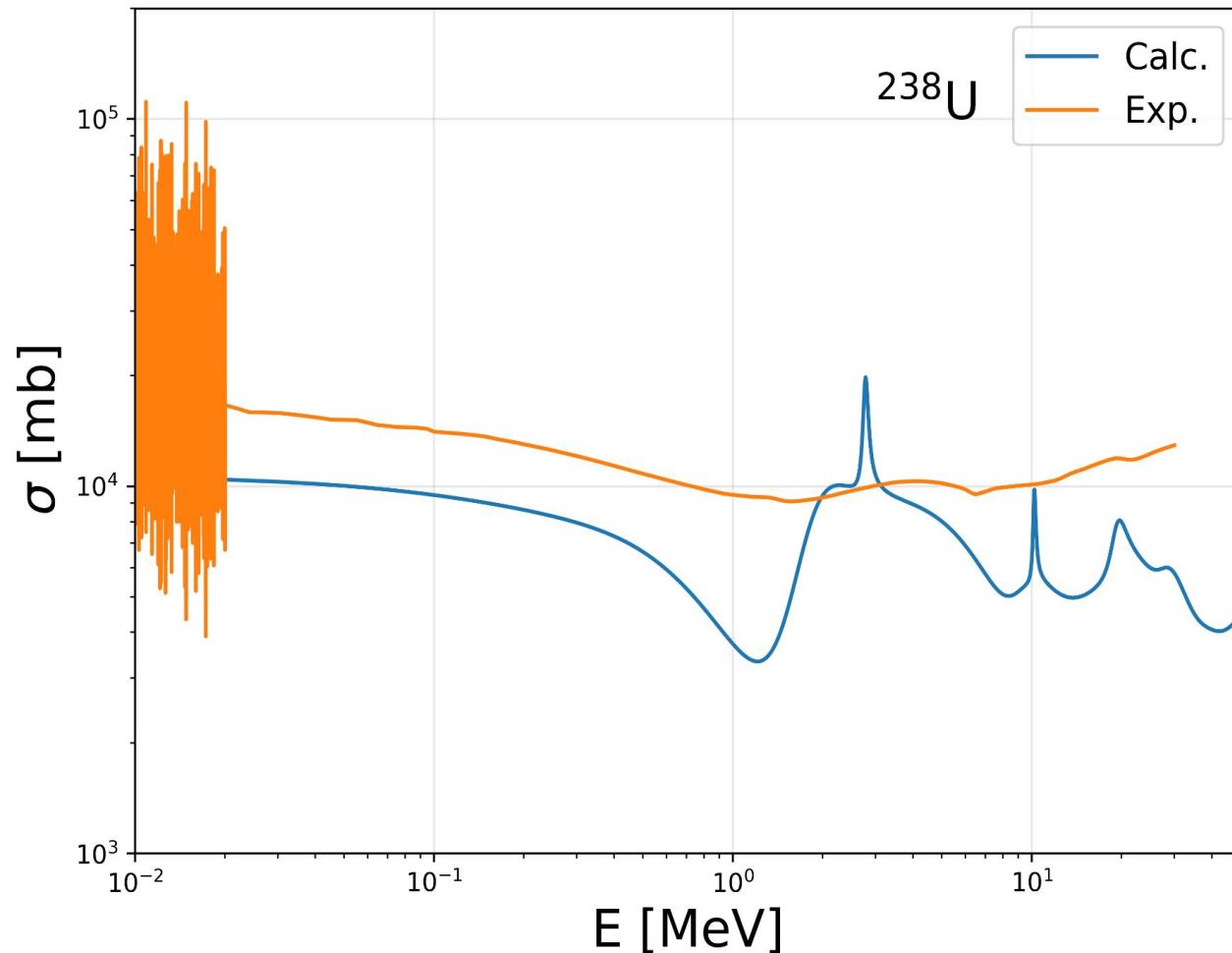
Sección transversal total ^{40}Ca



Sección transversal total ^{107}Ag



Sección transversal total ^{238}U



Conclusiones

Se obtienen desviaciones considerables entre el modelo computacional y las medidas experimentales debido probablemente a la las siguientes causas:

- Ignorancia del potencial exacto.
- Aproximaciones teóricas en el método de Numerov y de ondas parciales.
- Se simula la dispersión por un único núcleo, situación que experimentalmente no se realiza.
- Ruido del experimento.

Referencias

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¡GRACIAS!

