Fenómenos Colectivos en Sólidos – Pablo Tamborenea
Primer cuatrimestre 2021

Ejercicio 1 - guía 2
Transformada Fourier 3D
de potencial de Coulomb y de Yukawa

Máximo Riso

Intro

$$\nabla^2 \phi(\mathbf{r}) = -4\,\pi\,\rho(\mathbf{r})$$

Ec. Poisson

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Transformada de Fourier del potencial

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$$\hat{V}(\mathbf{k}) = \int_0^{\infty}\int_0^{2\pi}\int_0^{\pi} \frac{1}{r}\, e^{-i\,k\,r\,\cos(\theta)}\, r^2\, \sin(\theta)\, d\theta\, d\varphi\, dr$$

En coordenadas esféricas

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En coordenadas esféricas

$$\hat{V}(\mathbf{k}) = 2\pi \int_0^{\infty} \int_{-1}^{1} e^{-i\,k\,r\,u}\, r\, du\, dr$$

Sustituyendo u = cos (θ)

Integrando φ de 0 a 2 π

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$$\hat{V}(\mathbf{k}) = 2\pi \int_0^{\infty} \left(\frac{e^{-i\,k\,r\,u}\, r}{-ikr} \right) \Bigg|_{u=-1}^{u=1} dr$$

Integrando en u

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$$\hat{V}(\mathbf{k}) = 2\pi i \int_0^{\infty} \left(\frac{e^{-ikr}}{k} - \frac{e^{ikr}}{k} \right) dr$$

Evaluando

$$\hat{V}(\mathbf{k}) = 2\pi i \int_0^\infty \left(\frac{e^{-ikr}}{k} - \frac{e^{ikr}}{k} \right) dr$$

Problema: Integral irregular

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$$k = k_r - i\,k_I \qquad k = k_r + i\,k_I \qquad \text{donde } k_I > 0$$

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$$\hat{V}(\mathbf{k}) = 2\pi i \int_0^\infty \frac{e^{-i\,(k_R - ik_I)\,r}}{(k_R - ik_I)} - \frac{e^{i\,(k_R + ik_I)\,r}}{(k_R + ik_I)}\, dr$$

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Integrando

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||

$$\hat{V}(\mathbf{k}) = 2\pi \left(- \frac{e^{-i\,k_R\,r}\, e^{-\,k_I\,r}}{(k_R - ik_I)^2} - \frac{e^{k_R\,r}\, e^{-\,k_I\,r}}{(k_R + ik_I)^2} \right) \Big|_{r=0}^{r\to\infty}$$

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Integrando

$$||$$

$$\hat{V}(\mathbf{k}) = 2\pi \left(- \frac{e^{-i\,k_R\,r}\, e^{-\,k_I\,r}}{(k_R - ik_I)^2} - \frac{e^{\,k_R\,r}\, e^{-\,k_I\,r}}{(k_R + ik_I)^2}\right)\Bigg|_{r=0}^{r\to\infty}$$

$$\hat{V}(\mathbf{k}) = 2\pi \left(\frac{1}{(k_R - ik_I)^2} + \frac{1}{(k_R + ik_I)^2}\right)$$

Evaluando y
Tomando límite

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$k_I \rightarrow 0$

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Potencial de Coulomb

Transformada de Fourier del potencial

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← Planteamos la integral

$$\alpha = 1/\lambda$$

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En coordenadas esféricas

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En coordenadas esféricas

$$\hat{V}(\mathbf{k}) = 2\pi \int_0^\infty \int_{-1}^1 e^{-\alpha\, r}\, e^{-i\,k\,r\,u}\, r\, du\, dr$$

Sustituyendo $u = \cos(\theta)$

Integrando φ de 0 a 2π

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Integrando φ de 0 a 2π

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Integrando en u

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Evaluando

$$\hat{V}(\mathbf{k}) = 2\pi i \int_0^\infty \left(\frac{e^{-\alpha r}\, e^{-i k r}}{k} - \frac{e^{-\alpha r}\, e^{i k r}}{k}\right) dr$$

Observación: no es una integral irregular

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$$\hat{V}(\mathbf{k}) = 2\pi i \int_0^{\infty} \frac{e^{(-i k - \alpha) r}}{k} - \frac{e^{(i k - \alpha) r}}{k}\, dr$$

Reescribimos

$$\hat{V}(\mathbf{k}) = 2\pi i \int_0^\infty \left(\frac{e^{-\alpha r}\, e^{-i k r}}{k} - \frac{e^{-\alpha r}\, e^{i k r}}{k} \right) dr$$

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Integrando

$$\hat{V}(\mathbf{k}) = 2\pi i \int_0^{\infty} \left(\frac{e^{-\alpha r}\, e^{-i k r}}{k} - \frac{e^{-\alpha r}\, e^{i k r}}{k}\right) dr$$

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Integrando

$$\hat{V}(\mathbf{k}) = 2\pi i \left(\frac{1}{k(i k + \alpha)} + \frac{1}{k(i k - \alpha)}\right)$$

Tomando límite y evaluando

$$\hat{V}(\mathbf{k}) = 2\pi i \int_0^\infty \left(\frac{e^{-\alpha r}\, e^{-i k r}}{k} - \frac{e^{-\alpha r}\, e^{i k r}}{k}\right) dr$$

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Reescribiendo →

$$\hat{V}(\mathbf{k}) = 4\pi \frac{1}{(k^2 + \alpha^2)}$$

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$$\hat{V}(\mathbf{k}) = 4\pi \frac{1}{(k^2 + \alpha^2)}$$

$$\alpha = 1/\lambda$$

$$V_Y(\mathbf{r}) = -\frac{e^2}{\varepsilon\, r}\, e^{-r/\lambda}$$

→

$$\hat{V}_Y(\mathbf{k}) = -\frac{4\pi\, e^2}{\varepsilon\, (k^2 + (1/\lambda)^2)}$$

Potencial de Yukawa

Transformada de Fourier del potencial

Comparando

$$V_C(\mathbf{r}) = -\frac{e^2}{\varepsilon\, r}$$

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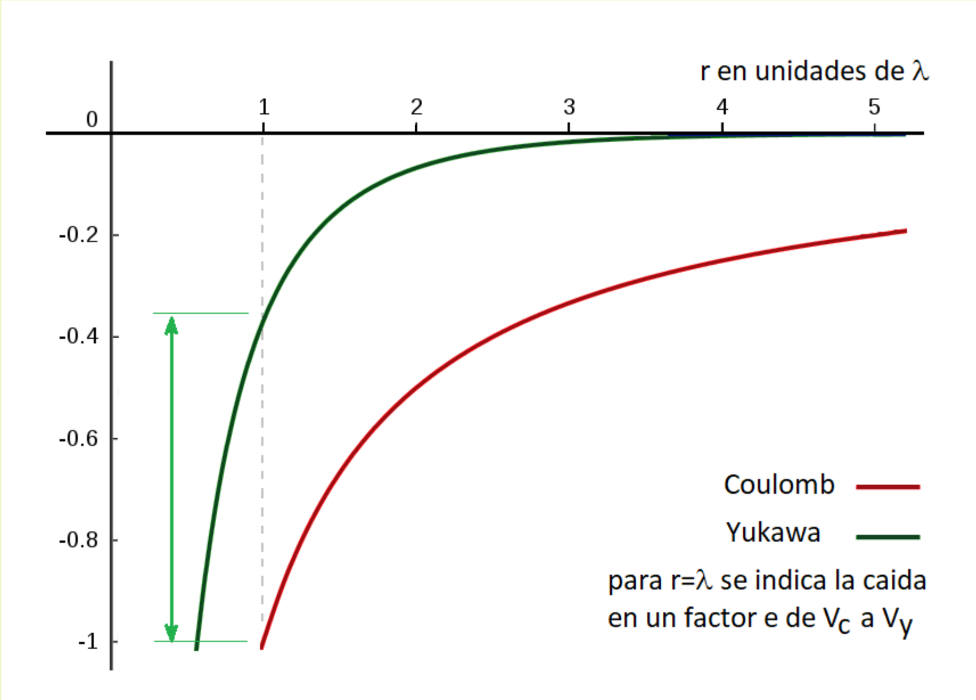

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Transformada

$$\hat{V}(\mathbf{k}) = 4\pi\, \frac{1}{(k^2 + \alpha^2)}$$

$$\hat{V}(\mathbf{k}) = \frac{4\pi}{k^2}\left(1 - \left(\frac{\alpha}{k}\right)^2 + \left(\frac{\alpha}{k}\right)^4 - \cdots\right)$$

Taylor

$$(\alpha/k)^2 << 1$$

Comparando

$$V_C(\mathbf{r}) = -\frac{e^2}{\varepsilon\, r}$$

Potencial Coulomb

$$\hat{V}_C(\mathbf{k}) = -\frac{4\pi\, e^2}{\varepsilon\, k^2}$$

Transformada

$$\hat{V}_Y(\mathbf{k}) = -\frac{4\pi\, e^2}{\varepsilon\, k^2}\left(1 - \left(\frac{1}{k\lambda}\right)^2 + \left(\frac{1}{k\lambda}\right)^4 - \cdots\right)$$

Taylor

$$k\lambda >> 1$$

$$V_Y(\mathbf{r}) = -\frac{e^2}{\varepsilon\, r}\, e^{-r/\lambda}$$

Potencial Yukawa

$$\hat{V}_Y(\mathbf{k}) = -\frac{4\pi\, e^2}{\varepsilon\,(k^2 + (1/\lambda)^2)}$$

Transformada

$$\hat{V}(\mathbf{k}) = 4\pi\,\frac{1}{(k^2+\alpha^2)}$$

$$\hat{V}(\mathbf{k}) = \frac{4\pi}{k^2}\left(1 - \left(\frac{\alpha}{k}\right)^2 + \left(\frac{\alpha}{k}\right)^4 - \cdots\right)$$

$$(\alpha/k)^2 << 1$$

Muchísimas gracias por su atención.
Espero no haberlos aburrido ¿Cuánto duró?

Sugerencias, comentarios o quejas a risomaximo@gmail.com