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ON SOME APPLICATIONS OF CONTACT POTENTIALS

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7th International Workshop on New Challenges in Quantum Mechanics: Integrability and Supersymmetry

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September 6, 2019

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2.- 1D non-relativistic $V(x) = -a\delta(x) + b\delta'(x)$

3.-
$$V(x) = \sum_{n=-\infty}^{\infty} \left(V_0 \,\delta(x - na) + aV_1 \,\delta'(x - na) \right)$$

4.- Radial potential: $V(r) = -a\delta(r - r_0) + b\delta'(r - r_0)$

5.- 3D: application in Nuclear Physics

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1.- INTRODUCTION

1D non-relativistic QM contact potentials are relevant in Theor. Phys.

Easy to deal with them to analyze basic quantum properties: bound states, resonances or scattering.

Used to model point defects in materials, thin structures, heterostructures (abrupt effective mass change), and topological insulators.

In nanophysics: to model sharply peaked impurities inside quantum dots.

in scalar QFT on a line: used to model impurities and external singular backgrounds.

Contact interactions $\delta(x)$ or $\delta'(x)$: analyze perturbations of a free kinetic Schrödinger Hamiltonian, the harmonic oscillator, a constant electric field, the infinite square well, the conical oscillator, etc.

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GENERAL PURPOSE:

The analysis of the 1D quantum Hamiltonian

$$H=\frac{p^2}{2m}-a\,\delta(x)+b\,\delta'(x),\quad a>0,\ b\in\mathbb{R}.$$

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Addition of extra terms of physical interest:

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If b = 0, we know:

1) *H* is self-adjoint in \mathcal{D} , continuous functions $\psi(x)$ such that

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2) There is a unique bound state $E = -\frac{ma^2}{2\hbar^2}$.

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On the meaning of $\delta'(x)$

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On the domain of self-adjointness for H

 $\psi(x) : \mathbb{R} \to \mathbb{C}$ in (Sobolev) space of continuous functions, except for a nite jump at the origin $(W_2^2(\mathbb{R}/\{0\}))$ such that: (i) $\psi(x) \in W_2^2(\mathbb{R}/\{0\}) \Rightarrow \psi'(x)$ continuous, except at the origin (ii) $\psi''(x)$ exists almost everywhere (iii) $\psi(x)$ and $\psi(x)''(x)$ are square integrable:

 $\sum_{-\infty}^{\infty} \{ |\psi(x)|^2 + |\psi''(x)|^2 \} \, dx < \infty \, .$

$$\begin{pmatrix} \psi(0^+) \\ \psi'(0^+) \end{pmatrix} = \begin{pmatrix} \frac{\hbar^2 + mb}{\hbar^2 - mb} & 0 \\ \frac{-2\hbar^2 am}{\hbar^4 - m^2 b^2} & \frac{\hbar^2 - mb}{\hbar^2 + mb} \end{pmatrix} \begin{pmatrix} \psi(0^-) \\ \psi'(0^-) \end{pmatrix}$$

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$$\int_{-\infty}^{\infty} \{|\psi(\mathbf{x})|^2 + |\psi''(\mathbf{x})|^2\} \, d\mathbf{x} < \infty \, .$$

$$\left(\begin{array}{c}\psi(0^{+})\\\psi'(0^{+})\end{array}\right) = \left(\begin{array}{c}\frac{\hbar^{2} + mb}{\hbar^{2} - mb} & 0\\\frac{-2\hbar^{2}am}{\hbar^{4} - m^{2}b^{2}} & \frac{\hbar^{2} - mb}{\hbar^{2} + mb}\end{array}\right) \left(\begin{array}{c}\psi(0^{-})\\\psi'(0^{-})\end{array}\right)$$

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THE SCHRÖDINGER EQUATION

For different values of E, we have to solve

$$-\frac{\hbar^2}{2m}\psi''-\mathbf{a}\,\delta(\mathbf{x})\psi(\mathbf{x})+\mathbf{b}\,\delta'(\mathbf{x})\psi(\mathbf{x})=E\psi(\mathbf{x})\,\ldots$$

We must properly define δ(x)ψ(x), δ'(x)ψ(x) as distributions
The δ'(x) term forces ψ(x) to be discontinuous at x = 0 (!!)

ACTION OF $\delta(\mathbf{x})$ and $\delta'(\mathbf{x})$ on discontinuous funct. Following Kurasov's proposal:

$$\psi(x)\delta(x) = \frac{\psi(0+) + \psi(0-)}{2}\,\delta(x)$$

 $\psi(x)\delta'(x) = rac{\psi(0+) + \psi(0-)}{2}\,\delta'(x) - rac{\psi'(0+) + \psi'(0-)}{2}\,\delta(x)\,.$
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BOUND SATES

Schrödinger equation with E < 0

As V(x) = 0 for $x \neq 0$, the solution that vanishes as $x \to \pm \infty$ is

$$\psi(x) = lpha e^{\kappa x} \Theta(-x) + eta e^{-\kappa x} \Theta(x), \quad \kappa = \sqrt{-2mE/\hbar^2},$$

where $\psi(0^-) = \alpha \neq \beta = \psi(0^+)$ and $\Theta(x)$ is the Heaviside step function.

To assure self-adjointness, we impose Kurasov's matching conditions:

$$E = -\frac{1}{2} \frac{ma^2 h^6}{(h^4 + b^2 m^2)^2}$$

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$$E = -rac{1}{2} \, rac{m a^2 \hbar^6}{(\hbar^4 + b^2 \, m^2)^2}$$

 $\psi(x) = \frac{\sqrt{ma\hbar}}{\hbar^4 + m^2 b^2} \left[(\hbar^2 - mb)e^{\kappa x} \Theta(-x) + (\hbar^2 + mb)e^{-\kappa x} \Theta(x) \right]$

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FIGURE: Energy of the only bound state as a function of *m b*



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T and R coefficients

INCOMING WAVE e^{ikx} , $k = \sqrt{2mE/\hbar^2}$, $E \ge 0$: For x < 0: $\psi(x) = e^{ikx} + Re^{-ikx}$ For x > 0: $\psi(x) = Te^{ikx}$ where *R* and *T* are the reflection and transmission coefficients Using the matching conditions at the origin:

$$\begin{pmatrix} T\\ ikT \end{pmatrix} = \begin{pmatrix} \frac{\hbar^2 + mb}{\hbar^2 - mb} & 0\\ \frac{-2am\hbar^2}{\hbar^4 - m^2b^2} & \frac{\hbar^2 - mb}{\hbar^2 + mb} \end{pmatrix} \begin{pmatrix} 1+R\\ ik(1-R) \end{pmatrix}$$

$$R(k) = \frac{-(am + 2mbk\,i)}{am + (1 + m^2b^2)k\,i}$$

$$T(k) = \frac{(1 - m^2 b^2)k i}{am + (1 + m^2 b^2)k i}$$

 $^{2} = 1$

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satisfying $|R(k)|^2 + |T(k)|^2 = 1$

 $(\hbar = 1)$

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T and R coefficients

INCOMING WAVE e^{ikx} , $k = \sqrt{2mE/\hbar^2}$, $E \ge 0$: For x < 0: $\psi(x) = e^{ikx} + Re^{-ikx}$ For x > 0: $\psi(x) = Te^{ikx}$ where *R* and *T* are the reflection and transmission coefficients Using the matching conditions at the origin:

$$\begin{pmatrix} T\\ ikT \end{pmatrix} = \begin{pmatrix} \frac{\hbar^2 + mb}{\hbar^2 - mb} & 0\\ \frac{-2am\hbar^2}{\hbar^4 - m^2b^2} & \frac{\hbar^2 - mb}{\hbar^2 + mb} \end{pmatrix} \begin{pmatrix} 1+R\\ ik(1-R) \end{pmatrix}$$

$$R(k) = \frac{-(am+2mbk\,i)}{am+(1+m^2b^2)k\,k}$$

$$T(k) = \frac{(1 - m^2 b^2) k i}{am + (1 + m^2 b^2) k i}$$

satisfying $|R(k)|^2 + |T(k)|^2 = 1$

 $(\hbar = 1)$

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The double $\delta - \delta'$ well JM Muñoz and J Mateos, PRD **91** (2015) 025028

Quantum vacuum interaction in a Casimir setup



by mimicking the plates as two contact interactions of the form:

 $H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + a_1\delta(x+q) + b_1\delta'(x+q) + a_2\delta(x-q) + b_2\delta'(x-q)$

Then, it is natural to consider ...

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3.- δ - δ' Dirac comb

Kronig-Penney model: exactly solvable periodic potential, used in Solid State Physics, which describes electron motion in a period array of **rectangular** barriers.

The **Dirac comb** is obtained by taking the appropriate limit in KP nodel, such that the rectangular barriers become Dirac delta distributions:

$$V_{DKP}(x) = V_0 \sum_{n=-\infty}^{\infty} \delta(x - na), \ V_0 > 0.$$

We consider a modified Dirac comb, adding a δ' in every singular point: $V_1(x) = \sum_{n=-\infty}^{\infty} \left(V_0 \,\delta(x - na) + aV_1 \,\delta'(x - na) \right), \ a, V_0 > 0, V_1 \in \mathbb{R}.$

Periodic array of charges and dipoles

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SOLVING THE QUANTUM MECHANICAL PROBLEM

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+V_1(x)\psi(x)=E\psi(x),$$

- First of all, we will solve Schrödinger equation in regions I and II
- Second, we will impose Kurasov's matching conditions at x = 0
- Finally, we will take into account Floquet-Bloch theorem

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Solving the Schrödinger Eqn. in regions *I* and *II*:

$$\psi_{I}(x) = A_{I} e^{ikx} + B_{I} e^{-ikx}, \qquad \psi_{II}(x) = A_{II} e^{ikx} + B_{II} e^{-ikx},$$
$$\psi_{I}'(x) = ikA_{I} e^{ikx} - ikB_{I} e^{-ikx}, \qquad \psi_{II}'(x) = ikA_{II} e^{ikx} - ikB_{II} e^{-ikx},$$
eing $k = \frac{\sqrt{2mE}}{\hbar} > 0.$

In matrix compact form:

$$ec{\psi}_J(x) = \left(egin{array}{c} \psi_J(x) \\ \psi_J'(x) \end{array}
ight) = \mathbb{KM}_x \left(egin{array}{c} A_J \\ B_J \end{array}
ight), \ J = I, II,$$

where

$$\mathbb{K} = \left(\begin{array}{cc} 1 & 1 \\ ik & -ik \end{array} \right), \qquad \mathbb{M}_x = \left(\begin{array}{cc} e^{ikx} & 0 \\ 0 & e^{-ikx} \end{array} \right)$$

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Solving the Schrödinger Eqn. in regions *I* and *II*:

$$\psi_{I}(x) = A_{I} e^{ikx} + B_{I} e^{-ikx}, \qquad \psi_{II}(x) = A_{II} e^{ikx} + B_{II} e^{-ikx},$$
$$\psi'_{I}(x) = ikA_{I} e^{ikx} - ikB_{I} e^{-ikx}, \qquad \psi'_{II}(x) = ikA_{II} e^{ikx} - ikB_{II} e^{-ikx},$$
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Solving the Schrödinger eqn. in regions I and II:

$$\begin{split} \psi_{l}(x) &= A_{l} e^{ikx} + B_{l} e^{-ikx}, & \psi_{ll}(x) &= A_{ll} e^{ikx} + B_{ll} e^{-ikx}, \\ \psi_{l}'(x) &= ikA_{l} e^{ikx} - ikB_{l} e^{-ikx}, & \psi_{ll}'(x) &= ikA_{ll} e^{ikx} - ikB_{ll} e^{-ikx}, \end{split}$$

being $k = \frac{\sqrt{2mE}}{\hbar} > 0$.

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Imposing the matching conditions at x = 0

Using the notation just introduced, Kurasov's matching conditions are

 $V_1 \neq \pm \hbar^2/(ma).$

They can be written as $\vec{\psi}_{II}(0^+) = \mathbb{T}_U \vec{\psi}_I(0^-)$, with

$$\mathbb{T}_{U} = \begin{pmatrix} \frac{1+U_{1}}{1-U_{1}} & 0\\ \frac{2U_{0}/a}{1-U_{1}^{2}} & \frac{1-U_{1}}{1+U_{1}} \end{pmatrix}, \ U_{0} = \frac{maV_{0}}{\hbar^{2}}, U_{1} = \frac{maV_{1}}{\hbar^{2}}$$

And finally

$$\left(\begin{array}{c}A_{ll}\\B_{ll}\end{array}\right) = \mathbb{K}^{-1}\mathbb{T}_{U}\mathbb{K}\left(\begin{array}{c}A_{l}\\B_{l}\end{array}\right).$$

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THE FLOQUET-BLOCH THEOREM

Now we must take into account the periodicity of the potential: the Floquet-Bloch theorem forces

$$\psi(x+a) = e^{iqa}\psi(x) \Rightarrow \psi'(x+a) = e^{iqa}\psi'(x)$$

where q is the momentum of the crystal.

In matrix form, for
$$x \in (-a, 0)$$
,

$$\vec{\psi}_{II}(x+a) = e^{iqa} \vec{\psi}_{I}(x) \Rightarrow \mathbb{KM}_{x}\mathbb{M}_{a} \left(\begin{array}{c} A_{II} \\ B_{II} \end{array} \right) = e^{iqa}\mathbb{KM}_{x} \left(\begin{array}{c} A_{I} \\ B_{I} \end{array} \right).$$

As the matrices \mathbb{M}_{x} and \mathbb{K} are invertible:

$$\mathbb{M}_{a}\mathbb{K}^{-1}\mathbb{T}_{U}\mathbb{K}-e^{iqa}\mathbb{I} igg| iggl(egin{array}{c} A_{l} \ B_{l} \end{pmatrix} =ec{\mathsf{0}},$$

and hence

$$\det\left[\mathbb{T}_{U}-e^{iqa}\mathbb{K}\mathbb{M}_{a}^{-1}\mathbb{K}^{-1}\right]=0.$$

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Now we must take into account the periodicity of the potential: the Floquet-Bloch theorem forces

$$\psi(\mathbf{x} + \mathbf{a}) = \mathbf{e}^{i\mathbf{q}\mathbf{a}}\psi(\mathbf{x}) \Rightarrow \psi'(\mathbf{x} + \mathbf{a}) = \mathbf{e}^{i\mathbf{q}\mathbf{a}}\psi'(\mathbf{x})$$

where q is the momentum of the crystal.

In matrix form, for $x \in (-a, 0)$,

$$\vec{\psi}_{II}(x+a) = e^{iqa} \vec{\psi}_I(x) \Rightarrow \mathbb{KM}_x \mathbb{M}_a \left(\begin{array}{c} A_{II} \\ B_{II} \end{array} \right) = e^{iqa} \mathbb{KM}_x \left(\begin{array}{c} A_I \\ B_I \end{array} \right).$$

As the matrices \mathbb{M}_{x} and \mathbb{K} are invertible:

$$[\mathbb{M}_{a}\mathbb{K}^{-1}\mathbb{T}_{U}\mathbb{K}-e^{iqa}\mathbb{I}] \begin{pmatrix} A_{l} \\ B_{l} \end{pmatrix} = \vec{0},$$

and hence

$$\det\left[\mathbb{T}_{U}-e^{iqa}\mathbb{K}\mathbb{M}_{a}^{-1}\mathbb{K}^{-1}\right]=0.$$

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THE DISPERSION RELATION:

Defining $\tilde{q} = aq$, $\tilde{k} = ka$, we get the dispersion relation (DR)

$$\boxed{\cos \tilde{\boldsymbol{q}} = f(\boldsymbol{U}_1) \left[\cos \tilde{\boldsymbol{k}} + \boldsymbol{U}_0 \ g(\boldsymbol{U}_1) \frac{\sin \tilde{\boldsymbol{k}}}{\tilde{\boldsymbol{k}}}\right]}$$

$$f(U_1) = \frac{1+U_1^2}{1-U_1^2}, \qquad g(U_1) = \frac{1}{1+U_1^2}$$

The DR is an even function of $U_1 \propto V_1$, the coefficient of δ' .

If there is no δ' -terms, then f(0) = g(0) = 1 and it reduces to the well now band structure of the standard Dirac comb

$$\cos ilde{q} = \cos ilde{k} + U_0 \, rac{\sin ilde{k}}{ ilde{k}}.$$

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ALLOWED (COLOR) AND FORBIDDEN (WHITE) BANDS

Case $U_0 = 0.1$:



Case $U_0 = 10$:



Case $U_0 = 1$:



Case $U_0 = 30$:



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4.- Hyperspherical δ - δ'

THE PROBLEM TO BE SOLVED:

A non-relativistic quantum particle in \mathbb{R}^d with hyper-spherical potential

 $\widehat{V}_{\delta \cdot \delta'}(r) = a\,\delta(r-r_0) + b\,\delta'(r-r_0), \quad a,b \in \mathbb{R}, \ r_0 > 0.$

The quantum Hamiltonian operator is

$$\mathbf{H} = \frac{-\hbar^2}{2 m} \widehat{\Delta}_d + \widehat{V}_{\delta - \delta'}(\mathbf{r}),$$

If we introduce dimensionless quantities:

$$\mathbf{h} \equiv \frac{2}{mc^2} \mathbf{H}, \quad w_0 \equiv \frac{2a}{\hbar c}, \quad w_1 \equiv \frac{bm}{\hbar^2}, \quad x \equiv \frac{mc}{\hbar} r$$

the dimensionless Hamiltonian reads

$$\mathbf{h} = -\Delta_d + w_0 \,\delta(x - x_0) + 2w_1 \,\delta'(x - x_0).$$

Use hyperspherical coordinates $(x, \Omega_d \equiv \{\theta_1, \dots, \theta_{d-2}, \phi\})$

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HYPERSPHERICAL COORDINATES

The *d*-dimensional Laplace operator Δ_d is

$$\Delta_{d} = \frac{1}{x^{d-1}} \frac{\partial}{\partial x} \left(x^{d-1} \frac{\partial}{\partial x} \right) + \frac{\Delta_{\mathcal{S}^{d-1}}}{x^2}$$

 $\Delta_{S^{d-1}} = -\mathbf{L}_d^2$ is the Laplace-Beltrami operator in S^{d-1} .

L_d^2 is the square of the generalised angular momentum operator.

he eigenvalue equation for **h** is separable in hyperspherical coordinates

$$\psi_{\lambda\ell}(x,\Omega_d) = R_{\lambda\ell}(x)Y_\ell(\Omega_d),$$

 $R_{\lambda\ell}(x)$ is the radial wave function.

$$\chi(d,\ell) \equiv -\ell(\ell+d-2).$$

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RADIAL PROBLEM:

The radial wave function is

$$\left[-\frac{d^2}{dx^2}-\frac{d-1}{x}\frac{d}{dx}+\frac{\ell(\ell+d-2)}{x^2}+V_{\delta\cdot\delta'}(x)\right]R_{\lambda\ell}(x)=\lambda R_{\lambda\ell},$$

being

$$V_{\delta \cdot \delta'}(x) = w_0 \delta(x - x_0) + 2w_1 \delta'(x - x_0)$$

We introduce the reduced radial function

$$u_{\lambda\ell}(x)\equiv x^{\frac{d-1}{2}}R_{\lambda\ell}(x),$$

to remove the first derivative, and we get

$$(\mathcal{H}_0 + V_{\delta \cdot \delta'}(x)) u_{\lambda \ell}(x) = \lambda_\ell u_{\lambda \ell}(x),$$

$$\mathcal{H}_0 \equiv -rac{d^2}{dx^2} + rac{(d+2\ell-3)(d+2\ell-1)}{4x^2}$$

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MATCHING CONDITIONS

The domain of the selfadjoint extension $\mathcal{H}_0 + V_{\delta \cdot \delta'}$ of the operator \mathcal{H}_0 defined on \mathbb{R}_{x_0} is given by the square integrable functions such that

$$\begin{pmatrix} f(x_0^+) \\ f'(x_0^+) \end{pmatrix} = \begin{pmatrix} \frac{1+w_1}{1-w_1} & 0 \\ \frac{w_0}{1-w_1^2} & \frac{1-w_1}{1+w_1} \end{pmatrix} \begin{pmatrix} f(x_0^-) \\ f'(x_0^-) \end{pmatrix}.$$

The matching conditions for the radial wave function $R_{\lambda\ell}$:

$$\begin{pmatrix} R_{\lambda\ell}(x_0^+) \\ R'_{\lambda\ell}(x_0^+) \end{pmatrix} = \begin{pmatrix} \alpha & 0 \\ \beta & \alpha^{-1} \end{pmatrix} \begin{pmatrix} R_{\lambda\ell}(x_0^-) \\ R'_{\lambda\ell}(x_0^-) \end{pmatrix},$$

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$$\alpha = \frac{1 + w_1}{1 - w_1},$$

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The solutions of the radial wave function is

$$R_{\kappa\ell}(x) = \begin{cases} A_1 \mathcal{I}_{\ell}(\kappa x) + B_1 \mathcal{K}_{\ell}(\kappa x) & \text{if } x \in (0, x_0), \\ A_2 \mathcal{I}_{\ell}(\kappa x) + B_2 \mathcal{K}_{\ell}(\kappa x) & \text{if } x \in (x_0, \infty), \end{cases}$$

where

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$$\mathcal{I}_{\ell}(z)\equiv rac{1}{z^{
u}} I_{\ell+
u}(z), \quad \mathcal{K}_{\ell}(z)\equiv rac{1}{z^{
u}} \mathcal{K}_{\ell+
u}(z) \quad ext{with} \quad
u\equiv rac{d-2}{2},$$

being I_{ℓ} and K_{ℓ} modified Bessel functions of the first and second kind. The matching conditions give the secular equation

$$F(\kappa x_0) = (d-2)(\alpha - \alpha^{-1}) + \beta x_0,$$

$$F(\kappa x_0) \equiv -\kappa x_0 \left(\frac{I_{\nu+\ell-1}(\kappa x_0)}{\alpha I_{\nu+\ell}(\kappa x_0)} + \frac{\alpha K_{\nu+\ell-1}(\kappa x_0)}{K_{\nu+\ell}(\kappa x_0)} \right) - (\alpha - \alpha^{-1}) \ell$$

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u}} I_{\ell+
u}(z), \quad \mathcal{K}_{\ell}(z)\equiv rac{1}{z^{
u}} \mathcal{K}_{\ell+
u}(z) \quad ext{with} \quad
u\equiv rac{d-2}{2},$$

being I_{ℓ} and K_{ℓ} modified Bessel functions of the first and second kind. The matching conditions give the secular equation

$$F(\kappa x_0) = (d-2)(\alpha - \alpha^{-1}) + \beta x_0,$$

$$F(\kappa x_0) \equiv -\kappa x_0 \left(\frac{I_{\nu+\ell-1}(\kappa x_0)}{\alpha I_{\nu+\ell}(\kappa x_0)} + \frac{\alpha K_{\nu+\ell-1}(\kappa x_0)}{K_{\nu+\ell}(\kappa x_0)} \right) - (\alpha - \alpha^{-1}) \ell$$

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The solutions of the radial wave function is

$$R_{\kappa\ell}(x) = \begin{cases} A_1 \mathcal{I}_{\ell}(\kappa x) + B_1 \mathcal{K}_{\ell}(\kappa x) & \text{if } x \in (0, x_0), \\ A_2 \mathcal{I}_{\ell}(\kappa x) + B_2 \mathcal{K}_{\ell}(\kappa x) & \text{if } x \in (x_0, \infty), \end{cases}$$

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BOUND STATES

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PLOTS:



FIGURE: Each curve represents $F(\kappa x_0)$ for different values of the angular momentum, and d = 2. The green horizontal line is the constant on the rhs. LEFT: $\alpha = 0.8$, $\beta = -3$ and $x_0 = 7$. RIGHT: $\alpha = -0.8$, $\beta = 3$ and $x_0 = 7$.

MORE:

- Scattering states
- Existence of zero modes (states of E = 0)

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5.- NUCLEAR PHYSICS

 δ - δ' interaction may be obtained as a limit of a regular mean-field nuclear potential with volume, surface, and spin-orbit parts:

$$H(\mathbf{r}) = -rac{\hbar^2}{2\mu}
abla_{\mathbf{r}}^2 + U_0(r) + U_{so}(r)(\mathbf{L}\cdot\mathbf{S}) + U_q(r)$$

 μ is the reduced. $U_0(r)$, $U_{so}(r)$, and $U_q(r)$ comes from Woods-Saxon:

$$U_{0}(r) = -V_{0} f(r) = -V_{0} \frac{1}{1 + e^{(r-R)/a}},$$

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RADIAL & ANGULAR PARTS:

The eigenfunction $\psi(\mathbf{r}) = \frac{u_{n\ell j}(r)}{r} \mathcal{Y}_{\ell jm}(\theta, \phi)$:

 ${}^{2}\mathcal{Y}_{\ell jm}(\theta,\phi) = \hbar^{2}\ell(\ell+1)\mathcal{Y}_{\ell jm}(\theta,\phi), \ (\mathbf{L}\cdot\mathbf{S})\mathcal{Y}_{\ell jm}(\theta,\phi) = \hbar^{2}\xi_{\ell,j}\mathcal{Y}_{\ell jm}(\theta,\phi)$

$$\xi_{\ell,j} \equiv \begin{cases} \frac{\ell}{2} & \text{for } j = \ell + \frac{1}{2}, \\ -\frac{(\ell+1)}{2} & \text{for } j = \ell - \frac{1}{2}, \end{cases} \quad \ell \in \mathbb{N} \cup \{\mathbf{0}\}.$$

 $\mathcal{V}_{\ell jm}(\theta, \phi)$ is a simultaneous eigenfunction of the operators

$$\mathbf{L}^2, \quad \mathbf{S}^2, \quad \mathbf{J}^2 = (\mathbf{L} + \mathbf{S})^2.$$

The 3D Schrödinger equation reduces to $H(\mathbf{r})\psi(\mathbf{r}) = E \psi(\mathbf{r})$ is

$$H(r) u_{n\ell j}(r) = E_{n\ell j} u_{n\ell j}(r)$$

 $H(r) = -\frac{\hbar^2}{2\mu} \left[\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} \right] - V_0 f(r) + V_{so} \xi_{\ell,j} f'(r) + V_q f''(r).$

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Limit $a \rightarrow 0$ in H(r):

$$\lim_{a\to 0} U_0(r) = -V_0 \lim_{a\to 0} f(r) = V_0 [\Theta(r-R) - 1], \qquad r \ge 0.$$

Consequently, we have that

$$\lim_{a\to 0} V_{so}\,\xi_{\ell,j}\,f'(r) = -V_{so}\,\xi_{\ell,j}\,\delta(r-R)\,.$$

And

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We get the following the singular Hamiltonian

 $H_{sing}(r) = -\frac{\hbar^2}{2\mu} \left[\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} \right] + V_0[\theta(r-R) - 1] - V_{so}\xi_{\ell,l}\,\delta(r-R) - V_q\delta'(r-R).$

Ve will use this radial 1D Hamiltonian to describe an atomic nucleus.

Advantage: $H_{sing}(r) u(r) = E_{n\ell j} u(r)$ can be solved exactly $\forall (\ell, j)$.

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Schrödinger equation for the singular potential

$$\frac{d^2 u(r)}{dr^2} + \left\{ \frac{2\mu E}{\hbar^2} - \frac{2\mu V_0}{\hbar^2} \left[\theta(r-R) - 1 \right] + \alpha \, \delta(r-R) + \beta \, \delta'(r-R) - \frac{\ell(\ell+1)}{r^2} \right\} u(r) = 0 \,,$$

where

$$lpha = rac{2\mu}{\hbar^2} V_{so}\,\xi_{\ell,j}, \qquad eta = rac{2\mu}{\hbar^2} V_q\,.$$

Wave equation inside the nucleus $(0 \le r < R)$: in this region the square integrable solution is

$$u_{1,\ell}(r) = A_\ell \sqrt{\gamma r} J_{\ell+\frac{1}{2}}(\gamma r), \quad \gamma = rac{\sqrt{2\mu(V_0+E)}}{\hbar}, \quad r \in [0,R).$$

$$u_{2,\ell}(r) = D_\ell \sqrt{\kappa r} K_{\ell+\frac{1}{2}}(\kappa r), \qquad \kappa := \frac{\sqrt{2\mu|E|}}{\hbar}, \quad r \in (R,\infty).$$

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MATCHING CONDITIONS AT r = R

To fix a self-adjoint extension of the relevant operator

$$\left(egin{array}{c} u_{2,\ell}(R^+) \ u_{2,\ell}'(R^+) \end{array}
ight) = \left(egin{array}{c} rac{2+eta}{2-eta} & 0 \ rac{4lpha}{4-eta^2} & rac{2-eta}{2+eta} \end{array}
ight) \left(egin{array}{c} u_{1,\ell}(R^-) \ u_{1,\ell}'(R^-) \end{array}
ight),$$

From here, the secular equation

$$\frac{\chi J_{\ell+\frac{3}{2}}(\chi)}{J_{\ell+\frac{1}{2}}(\chi)} = \frac{(2+\beta)^2}{(2-\beta)^2} \frac{\sigma K_{\ell+\frac{3}{2}}(\sigma)}{K_{\ell+\frac{1}{2}}(\sigma)} - \frac{8\beta(\ell+1)}{(2-\beta)^2} + \frac{w_0}{(2-\beta)^2} = \phi(\sigma),$$

/here

$$\chi := v_0 \sqrt{1-\varepsilon} \,, \qquad \sigma := v_0 \sqrt{\varepsilon} \,,$$

$$\begin{split} v_0 &\equiv \sqrt{\frac{2\mu R^2 V_0}{\hbar^2}} > 0, \quad w_0 \equiv 4\alpha R = \frac{8\mu V_{so}\xi_{\ell,j}R}{\hbar^2}, \\ \varepsilon &\equiv \frac{|E|}{V_0} \in (0,1). \end{split}$$

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MATCHING CONDITIONS AT r = R

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PHYSICAL EXAMPLE

For the isotope ²⁰⁹Pb, the relevant parameters describing the lowest experimental energy states are

$$V_0 = 44.4 \text{ MeV}, V_{so} = 16.5 \text{ MeV} \text{ fm}, R = 7.525 \text{ fm},$$

a = 0.7 fm, and $\frac{2\mu}{\hbar^2} = 0.0480253$ MeV⁻¹ fm⁻².

Then:
$$v_0 = 10.98$$
, $w_0 = 23.83 \xi_{\ell,j}$.

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Then:
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			$\beta = 1$	
State	Numerical	Model	Numerical	Model
	-41.35	-41.36	-40.97	-40.85
1 <i>s</i> _{1/2}	-32.27	-32.31	-31.11	-30.23
2 <i>s</i> _{1/2}	-17.53	-17.61	-18.11	-12.92
0 <i>p</i> _{3/2}	-38.21	-37.96	-37.48	-37.12
$1p_{3/2}$	-26.29	-25.53	-25.30	-22.97
2p _{3/2}	-9.17	-7.71	-13.30	-2.78
0 <i>p</i> _{1/2}	-38.08	-39.16	-37.34	-37.19
$1p_{1/2}$	-25.91	-28.57	-24.44	-23.32
2p _{1/2}	-8.47	-12.48	-11.20	-5.74

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	$\beta = 0$		$\beta = 1$	
State	Numerical	Model	Numerical	Model
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RESONANCES:

Resonance state functions (Gamow functions) are not square integrable.

We may write this solution for r > R in terms of the Hänkel functions f first (1) and second kind (2) as

$$u_l(r) := \sqrt{\kappa r} \left(C_{\ell} H_{\ell+\frac{1}{2}}^{(1)}(\kappa r) + \mathbf{D}_{\ell} H_{\ell+\frac{1}{2}}^{(2)}(\kappa r) \right), \ \kappa = \frac{\sqrt{2\mu E}}{\hbar}, \ E > 0.$$

Resonances are given by the **purely outgoing boundary condition**: only the outgoing wave function survives.

Asymptotic behavior: $H_{\ell+\frac{1}{2}}^{(1)}(\kappa r)$ is outgoing; $H_{\ell+\frac{1}{2}}^{(2)}(\kappa r)$ is incoming. This is condition is satisfied if and only if $D_{\ell} = 0$. Imposing the matching condition between the outgoing function and the wave function inside the potential well (nucleus):

$$\begin{split} H^{(1)}_{\ell+\frac{1}{2}}(R\kappa) &\left[8(\alpha R - \beta) J_{\ell+\frac{1}{2}}(R\gamma) - (\beta - 2)^2 R\gamma J_{\ell+\frac{3}{2}}(R\gamma) + (\beta - 2)^2 R\gamma J_{\ell-\frac{1}{2}}(R\gamma) \right] \\ &+ (\beta + 2)^2 \kappa R J_{\ell+\frac{1}{2}}(R\gamma) H^{(1)}_{\ell+\frac{3}{2}}(R\kappa) - (\beta + 2)^2 \kappa R J_{\ell+\frac{1}{2}}(R\gamma) H^{(1)}_{\ell-\frac{1}{2}}(R\kappa) \end{split}$$

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- Resonances

TYPES OF SOLUTIONS:

- (i) Simple solutions on the positive imaginary axis that correspond to the **bound states**.
- (ii) Simple solutions on the negative part of the imaginary axis, that show the presence of **antibound or virtual states**.
- (iii) Pairs of solutions on the lower half plane, symmetrically located with respect to the imaginary axis: **resonances**.

LM Nieto

Summary

1 Introduction

- $2 \delta(x) \& \delta'(x)$ Overview
- Bound sates T and R coeff Two $\delta \cdot \delta'$ wells

 $3 \delta - \delta'$ Dirac comb

4 Radial $\delta - \delta'$

The problem Radial problem Matching condition: Bound states

5 Nuclear Physics

Mean-field potential Sol. singular eqn. Matching conditions at r = R

Physical exampl

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PLOTS: In blue $P_{0} = F(k, k)$ and in red

In blue Re $F(k_1, k_2) = 0$ and in red Im $F(k_1, k_2) = 0$, from the key equation. Bound states and resonances correspond to intersection of red and blue curves. The parameters are $v_0 = 5$, $w_0 = 10$ and $\beta = 1$.

 $\ell = 0$:



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More plots: $\ell = 1, 2, 3, 4$



