DIRAC-COULOMB HAMILTONIANS

JAN DEREZIŃSKI

Department of Mathematical Methods in Physics

FACULTY OF PHYSICS

UNIVERSITY OF WARSAW

in collaboration with BŁAŻEJ RUBA from Jagiellonian University

A relativistic electron in the Coulomb potential is described by the Dirac-Coulomb Hamiltonian

$$\sum_{j=1}^{3} \alpha_j p_j + \beta m - \frac{\lambda}{|x|},$$

acting on spinor-valued functions on $\mathbb{R}^3$. Here α_i, β are Dirac matrices.

It is tricky and often ambiguous to interpret this expression as a self-adjoint operator. Physical properties, e.g. eigenvalues depend on the choice of a self-adjoint realization.

The usual approach to unbounded Hermitian operators is to find a domain on which they are essentially self-adjoint. Then our operator extends to a unique self-adjoint realization. Such an approach works e.g. for the Schrödinger-Coulomb Hamiltonian

$$-\Delta - \frac{\lambda}{|x|},$$

where the essential self-adjointness on $C_{\mathrm{c}}^{\infty}(\mathbb{R}^3)$ follows for any $\lambda \in \mathbb{R}$ by the famous Kato-Rellich Theorem.

The situation is much more complicated for Dirac-Coulomb Hamiltonians. There exists a very large mathematical literature about self-adjoint realizations of Dirac-Coulomb Hamiltonians (Kato, Gustaffson-Rejtö, Schmincke, Wüst, Klaus, Nenciu, Esteban-Loss....)

- Direct application of the Kato-Rellich Theorem yields essential self-adjointness for $|\lambda| < \frac{1}{2}$.
- More refined methods extend this to $|\lambda| \leq \frac{\sqrt{3}}{2}$.
- For $\frac{\sqrt{3}}{2} < |\lambda|$ essential self-adjointness breaks down.
  - For $\frac{\sqrt{3}}{2} < |\lambda| < 1$ there are two distinguished self-adjoint realizations, one of them "more physical".
  - For $|\lambda| = 1$ there is only one distinguished s.a. realization.
  - For $|\lambda| > 1$ there are no distinguished s.a. realizations.

I would like to describe an approach to Dirac-Coulomb Hamiltonians that in my opinion clarifies the concept of a "distinguished self-adjoint realization", based on my recent work with Błażej Ruba. The key elements of our approach are the homogeneity and the holomorphy.

First note that the mass term is bounded and thus does not change the domain of self-adjoint realizations and can be dropped.

Note also that dimension $d = 3$ is not important, and we can consider the Dirac-Coulomb Hamiltonian in any dimension

$$\sum_{i=1}^{d} \alpha_i p_i - \frac{\lambda}{|x|}.$$

The d-dimensional Dirac-Coulob Hamiltonian commutes with

$$\beta\Big(\sum_{i<j}\alpha_i\alpha_j(x_ip_j - x_jp_i) + \frac{d-1}{2}\Big),$$

which is essentially the Dirac operator on the sphere $\mathbb{S}^{d-1}$. Its eigenvalues are

$$\pm\omega \in \{0,1,2,\dots\} + \frac{d-1}{2}.$$

Thus after separation of angular variables we obtain the 1-dimensional Dirac-Coulomb Hamiltonian

$$D_{\omega,\lambda} := \begin{bmatrix} -\frac{\lambda+\omega}{x} & -\partial_x \\ \partial_x & -\frac{\lambda-\omega}{x} \end{bmatrix}.$$

Henceforth we will analyze $D_{\omega,\lambda}$ as an operator on $L^2(\mathbb{R}_+,\mathbb{C}^2)$. We will allow ω,λ to be complex.

The theory of the Dirac-Coulomb Hamiltonian is closely related to the Whittaker equation (related to the confluent hypergeometric equation)

$$\Big(-\partial_z^2+\Big(m^2-\frac{1}{4}\Big)\frac{1}{z^2}-\frac{\beta}{z}+\frac{1}{4}\Big)g=0.$$

There are two kinds of Whittaker functions, which are its solutions

$$\mathcal{I}_{\beta,m}(z)\simeq\frac{z^{\frac{1}{2}+m}}{\Gamma(1+2m)},\quad z\to0;$$
$$\mathcal{K}_{\beta,m}(z)\simeq z^{\beta}\mathrm{e}^{-\frac{z}{2}},\qquad z\to+\infty.$$

For $|\mathrm{Re}\sqrt{\omega^2-\lambda^2}|\geq\frac{1}{2}$ the operator $D_{\omega,\lambda}$ has only one closed realisation (this will be explained later). In particular, if ω,λ are real, then it is essentially self-adjoint on $C_{\mathrm{c}}^{\infty}(\mathbb{R}_+,\mathbb{C}^2)$. It is homogeneous of degree -1.

Let $k \in \mathbb{C}\backslash\mathbb{R}$ and consider the resolvent of the Dirac-Coulomb Hamiltonian $(D_{\omega,\lambda} - k)^{-1}$. Its integral kernel can be computed:

$$\begin{aligned}
G_{\omega,\lambda}(k;x,y) &= -\theta(y-x)\xi^{\pm}_{\omega,\lambda}(k,x)\zeta^{\pm}_{\omega,\lambda}(k,y)^{\mathrm{T}} \\
&\qquad -\theta(x-y)\zeta^{\pm}_{\omega,\lambda}(k,x)\xi^{\pm}_{\omega,\lambda}(k,y)^{\mathrm{T}}, \qquad k \in \mathbb{C}_{\pm}; \\
\xi^{\pm}_{\omega,\lambda}(k,x) &= \frac{\Gamma(1+\mu\mp\mathrm{i}\lambda)}{2\mu(\omega-\lambda\mp\mathrm{i}\mu)}\Bigg(\mp\mathrm{i}\omega\mathcal{I}_{\pm\mathrm{i}\lambda,\mu+\frac{1}{2}}(\mp 2\mathrm{i}kx)\begin{bmatrix}\omega-\lambda\\ \mu\end{bmatrix} \\
&\qquad + \mathcal{I}_{\pm\mathrm{i}\lambda,\mu-\frac{1}{2}}(\mp 2\mathrm{i}kx)\begin{bmatrix}\omega-\lambda\\ -\mu\end{bmatrix}\Bigg), \\
\zeta^{\pm}_{\omega,\lambda}(k,x) &= \frac{\omega\,\mathcal{K}_{\pm\mathrm{i}\lambda,\mu+\frac{1}{2}}(\mp 2\mathrm{i}kx)}{\mu(\omega-\lambda\pm\mathrm{i}\mu)}\begin{bmatrix}\omega-\lambda\\ \mu\end{bmatrix} \\
&\qquad + \frac{(\lambda\mp\mathrm{i}\mu)\mathcal{K}_{\pm\mathrm{i}\lambda,\mu-\frac{1}{2}}(\mp 2\mathrm{i}kx)}{\mu(\omega-\lambda\pm\mathrm{i}\mu)}\begin{bmatrix}\omega-\lambda\\ -\mu\end{bmatrix}.
\end{aligned}$$

where $\mu := \sqrt{\omega^2 - \lambda^2}$.

Let us try to understand what happens in the region $|\mathrm{Re}\sqrt{\omega^2-\lambda^2}|<\frac{1}{2}$. To this end, we check that the space of zero energy eigenfunctions of $D_{\omega,\lambda}$ is spanned by

$$\frac{x^{\mu}}{\omega+\lambda}\begin{bmatrix}-\mu\\ \omega+\lambda\end{bmatrix},\quad \frac{x^{-\mu}}{\omega+\lambda}\begin{bmatrix}\mu\\ \omega+\lambda\end{bmatrix},$$

with $\mu^2=\omega^2-\lambda^2$. Both eigenfunctions are square integrable near 0 if and only if $|\mathrm{Re}\sqrt{\omega^2-\lambda^2}|<\frac{1}{2}$.

One can introduce the maximal domain of $D_{\omega,\lambda}$:

$$\mathcal{D}_{\omega,\lambda}^{\max}:=\{f\in L^2\ :\ D_{\omega,\lambda}f\in L^2\},$$

and the minimal domain $\mathcal{D}_{\omega,\lambda}^{\min}$, which is the closure of C_{c} in the graph norm of $D_{\omega,\lambda}$. Clearly, $\mathcal{D}_{\omega,\lambda}^{\min}\subset\mathcal{D}_{\omega,\lambda}^{\max}$.

One can show the following

Lemma. If $|\mathrm{Re}\sqrt{\omega^2-\lambda^2}| \geq \frac{1}{2}$, then $\mathcal{D}_{\omega,\lambda}^{\min} = \mathcal{D}_{\omega,\lambda}^{\max}$,
If $|\mathrm{Re}\sqrt{\omega^2-\lambda^2}| < \frac{1}{2}$, then $\dim \mathcal{D}_{\omega,\lambda}^{\max}/\mathcal{D}_{\omega,\lambda}^{\min} = 2$.

Thus in the region $|\mathrm{Re}\sqrt{\omega^2-\lambda^2}| < \frac{1}{2}$ we have the following closed realizations of $D_{\omega,\lambda}$: the minimal, maximal and a one-parameter family given by the following boundary conditions near zero depending on $\kappa \in \mathbb{C} \cup \{\infty\}$:

$$\simeq \frac{x^{\mu}}{\omega+\lambda}\begin{bmatrix} -\mu \\ \omega+\lambda \end{bmatrix} + \kappa\frac{x^{-\mu}}{\omega+\lambda}\begin{bmatrix} \mu \\ \omega+\lambda \end{bmatrix}.$$

Let us go back to the region $|\mathrm{Re}\sqrt{\omega^2-\lambda^2}| \geq \frac{1}{2}$, where $D_{\omega,\lambda}$ has a unique closed realization, whose resolvent we computed in terms of Whittaker functions. It is easy to see that this resolvent can be analytically continued in ω, λ inside the region $|\mathrm{Re}\sqrt{\omega^2-\lambda^2}| < \frac{1}{2}$. Thus we obtain an analytic family of Dirac-Coulomb Hamiltonians.

This family cannot be unambiguously parametrized by ω, λ, because of two square roots of

$$\mu^2 = \omega^2 - \lambda^2.$$

One can try to parametrize it by the set

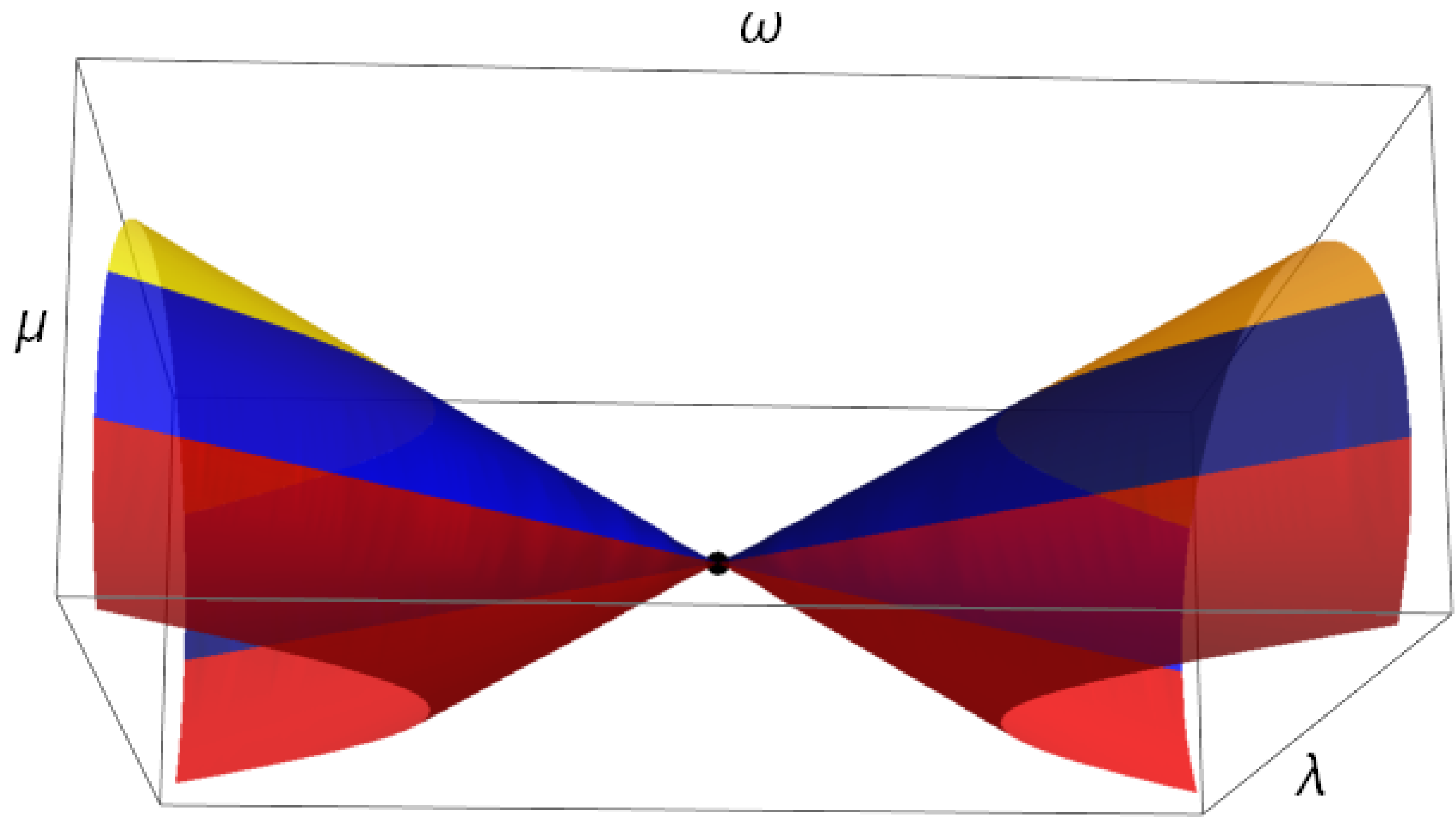
$$\Big\{(\omega, \lambda, \mu) \;:\; \mu^2 = \omega^2 - \lambda^2, \quad \mathrm{Re}\mu > -\frac{1}{2}\Big\},$$

but there is still a problem at $(\omega, \lambda, \mu) = (0, 0, 0)$, where the above manifold has a singularity.

The correct parameter space involves blowing-up this singularity. It is an everywhere holomorphic manifold, denoted $\mathcal{M}_{-\frac{1}{2}}$, and can be described as follows:

$$\left\{(\omega,\lambda,\mu,[a:b])\in\mathbb{C}^3\times\mathbb{CP}^1 \mid \begin{bmatrix}\omega+\lambda & \mu\\ \mu & \omega-\lambda\end{bmatrix}\begin{bmatrix}a\\ b\end{bmatrix}=\begin{bmatrix}0\\ 0\end{bmatrix},\ \mathrm{Re}\mu>-\frac{1}{2}\right\}.$$

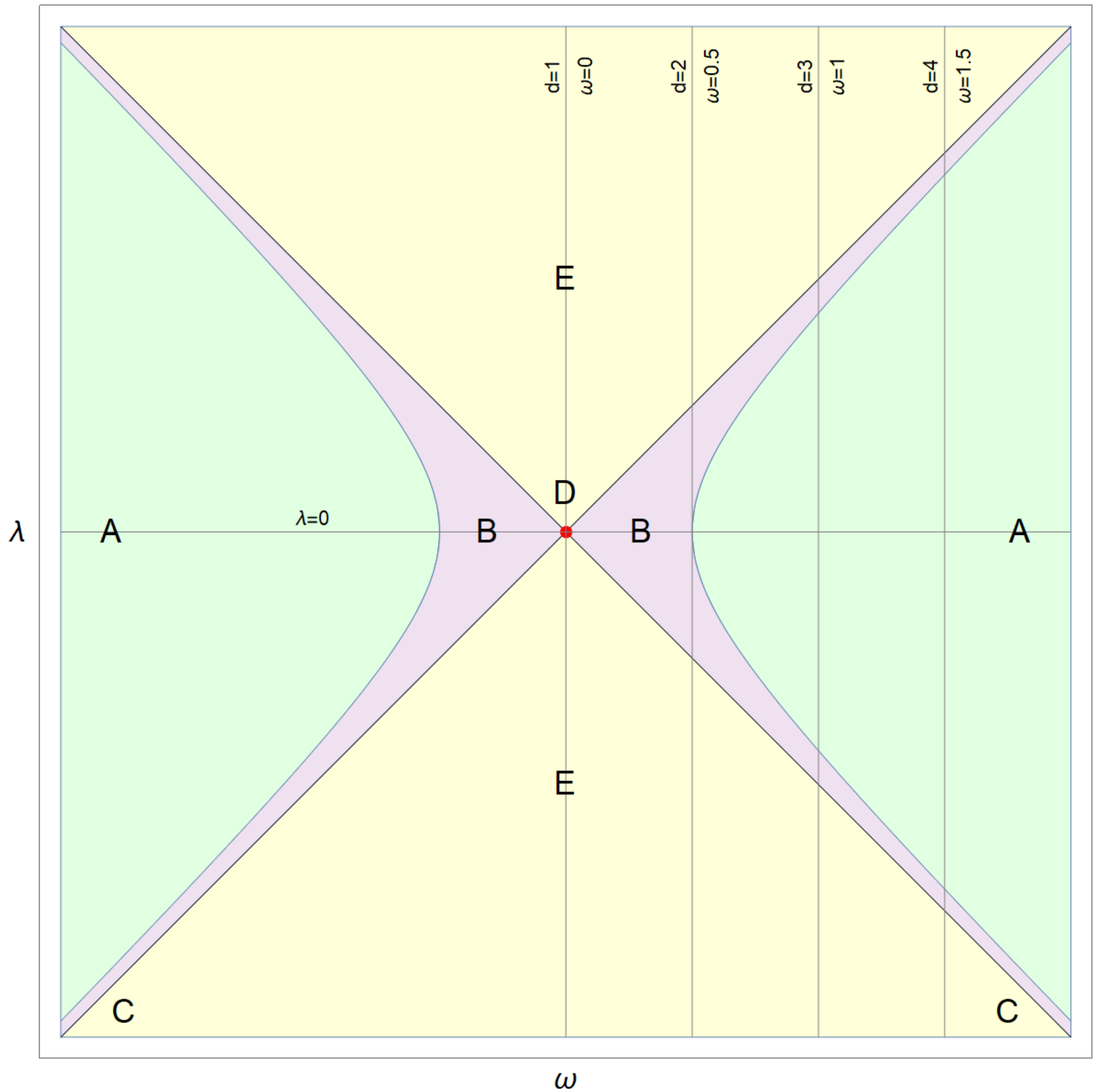
Thus we obtain a holomorphic family of homogeneous Dirac-Coulomb Hamilitonians $\mathcal{M}_{-\frac{1}{2}}\ni p\mapsto D_p$. The elements of this family have homogeneous boundary conditions $\simeq x^{\mu}$.



Parameter manifold $\mathcal{M}_{-\frac{1}{2}}$. Regions colored yellow, blue and red are described by inequalities $\mu > \frac{1}{2}$, $0 < \mu < \frac{1}{2}$ and $-\frac{1}{2} < \mu < 0$, respectively.

On the next slide we show the phase diagram of operators $D_{\omega,\lambda}$ for $(\omega, \lambda) \in \mathbb{R}^2$. We distinguish the following phases marked with different colors and letters:

$$
\begin{array}{ll}
A & \dfrac{1}{4} \leq \omega^2 - \lambda^2, \\
B & 0 < \omega^2 - \lambda^2 < \dfrac{1}{4}, \\
C & \omega = \pm\lambda, \quad (\omega, \lambda) \neq (0, 0), \\
D & (\omega, \lambda) = (0, 0), \\
E & \omega^2 - \lambda^2 < 0.
\end{array}
$$

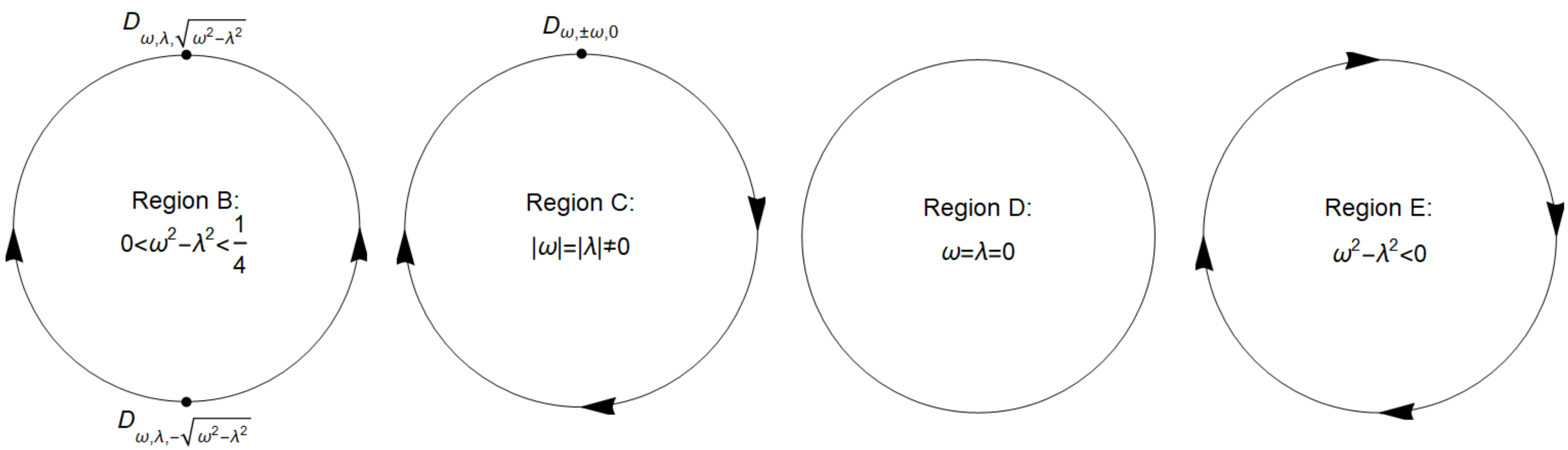


d=1
ω=0
d=2
ω=0.5
d=3
ω=1
d=4
ω=1.5
E
D
λ
A
λ=0
B
B
A
E
C
C
ω

Let $U_\tau f(x) = \mathrm{e}^{\frac{\tau}{2}} f(\mathrm{e}^\tau x)$ be the scaling transformation. The map

$$A \mapsto \mathrm{e}^\tau U_\tau A U_{-\tau}$$

will be called the renormalization group. Operators homogeneous of degree -1, such as the homogeneous Dirac-Coulomb Hamiltonians, are fixed points of this transformation.



The spectrum of self-adjoint homogeneous Dirac-Coulomb Hamiltonians is always $\mathbb{R}$. They can be diagonalized with help of two Møller operators

$$\begin{aligned}\mathcal{U}_p^{\pm} :&L^2(\mathbb{R}_+, \mathbb{C}^2) \to L^2(\mathbb{R}),\\ (\mathcal{U}_p^{\pm} D_p f)(k) &= k(\mathcal{U}_p^{\pm} f)(k), \qquad k \in \mathbb{R}.\end{aligned}$$

They can be derived from long-range scattering theory and are unitary for self-adjoint D_p. The two choices $\pm$ correspond to the incoming and outgoing waves. They are linked by the scattering amplitude

$$\begin{aligned}\mathcal{U}_p^{+} &= \mathrm{e}^{-\mathrm{i}\varepsilon_k \pi\mu} S_p \mathcal{U}_p^{-},\\ S_p &= \frac{(\omega - \lambda + \mathrm{i}\mu)\Gamma(1 + \mu - \mathrm{i}\lambda)}{(\omega - \lambda - \mathrm{i}\mu)\Gamma(1 + \mu + \mathrm{i}\lambda)}, \qquad \varepsilon_k := \mathrm{sgn}(k).\end{aligned}$$

One can explicitly express the Møller operators in terms of the generator of dilations $A := \frac{1}{2}(xp + px)$ and the hypergeometric function:

$$\Xi_p^{\pm}(\varepsilon_k, s) := \frac{\mathrm{i}^{\mp\varepsilon_k\mu - \frac{3}{2} - \mu + \mathrm{i}s} 2^{\mu-1}\Gamma(1+\mu\mp\mathrm{i}\lambda)}{\mu(z\pm\mathrm{i})}$$
$$\times\left(2\varepsilon_k\omega\Gamma\left(\frac{3}{2}+\mu-\mathrm{i}s\right){}_2\mathbf{F}_1\left(1+\mu+\mathrm{i}\varepsilon_k\lambda, \tfrac{3}{2}+\mu-\mathrm{i}s; 2\mu+2; 2+\mathrm{i}0\right)\begin{bmatrix}-z\\1\end{bmatrix}\right.$$
$$\left.+\,\mathrm{i}\,\Gamma\left(\frac{1}{2}+\mu-\mathrm{i}s\right){}_2\mathbf{F}_1\left(\mu+\mathrm{i}\varepsilon_k\lambda, \tfrac{1}{2}+\mu-\mathrm{i}s; 2\mu; 2+\mathrm{i}0\right)\begin{bmatrix}z\\1\end{bmatrix}\right),$$

$$\mathcal{U}_p^{\pm} = \frac{\mathrm{e}^{\frac{1}{2}\varepsilon_k\pi\lambda}}{\sqrt{\pi}}\Xi_p^{\pm\mathrm{T}}(\varepsilon_k, A)J,$$

$$z = -\frac{\mu}{\omega+\lambda} = -\frac{\omega-\lambda}{\mu}, \qquad (Jf)(k) = \frac{1}{k}f\Big(\frac{1}{k}\Big).$$

$\mathcal{U}_p^{\pm}$ can be extended analytically to complex ω, λ. However it stays bounded only for real λ. More precisely

$$\mathcal{U}_p^{\pm}(1 + A^2)^{-\frac{1}{2}|\mathrm{Im}(\lambda)|}$$

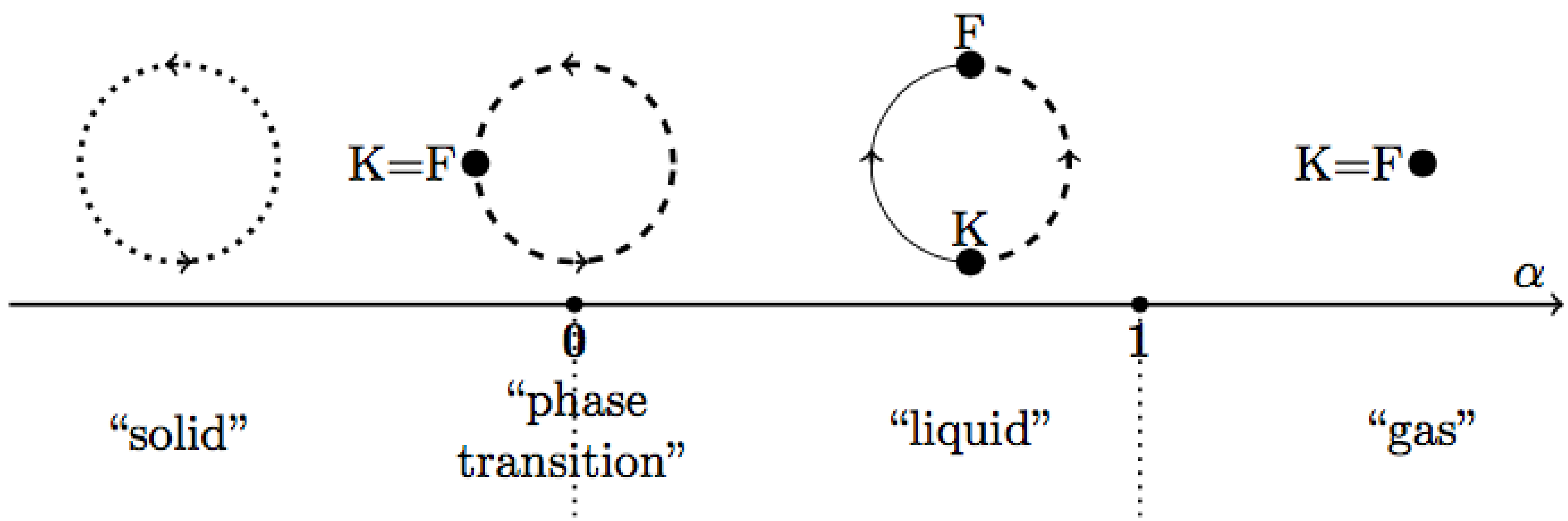
is bounded.

This is an expression of the fact that the angular momentum perturbation involving ω is effectively short range unlike the Coulomb potential multiplied by λ, which is long range (even though both decay as $\frac{1}{r}$).

A similar picture for the Bessel operator

$$L_\alpha = -\partial_x^2 + \big(-\frac{1}{4} + \alpha\big)\frac{1}{x^2}.$$

In particular, here is the phase diagram of its self-adjoint extensions:



K—Krein, F—Friedrichs, dashed line—single bound state, dotted line—infinite sequence of bound states.

MESSAGES:

1. There may be problems with strongly charged ions.
2. Boundary conditions can be tricky.
3. Homogeneous objects have special properties.
4. It is useful to organize things in holomorphic families.
5. Simple mathematical objects may have unexpected "phase transitions".

THANK YOU FOR YOUR ATTENTION