Spectral problems for quantum systems of particles with zero-range interactions

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Presentation given on 10 November 2022
at the Erwin Schrödinger Institute, Vienna

Quantum systems of particles
with zero-range ('contact') interaction
and their spectra

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two modern motivations:

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1) astrophysics: neutron scattering in neutron stars
2) cold atom physics: Fermi gases 'at unitarity', BCS/BEC crossover

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motivations from the past:

1930's: jump from atomic to nuclear physics (tritium): Wigner, Bethe, Peierls, Thomas, Fermi, Breit
1950's: models theoretical nuclear physics: Landau, Ter-Martirosyan, Skornyakov, Danilov, Gribov, ...
1960's: maths playgrounds for renormalisation and extension theory: Berezin, Faddeev, Birman, Minlos, ...
1960's-1970's: non-relativistic limit of QFT, φ_2^4, φ_3^4: Lee, Dimock, Hepp, Albeverio, Høegh-Krohn, ...
1970's: idealised solvable models (explicit computations / numerics): Demkov, Ostrovskii, Faddeev, Efimov, ...
1970's-1980's: universal low energy behaviour, renormalisation, resolvent approximation: Albeverio, Høegh-Krohn, Gesztesy, ...

(and others)

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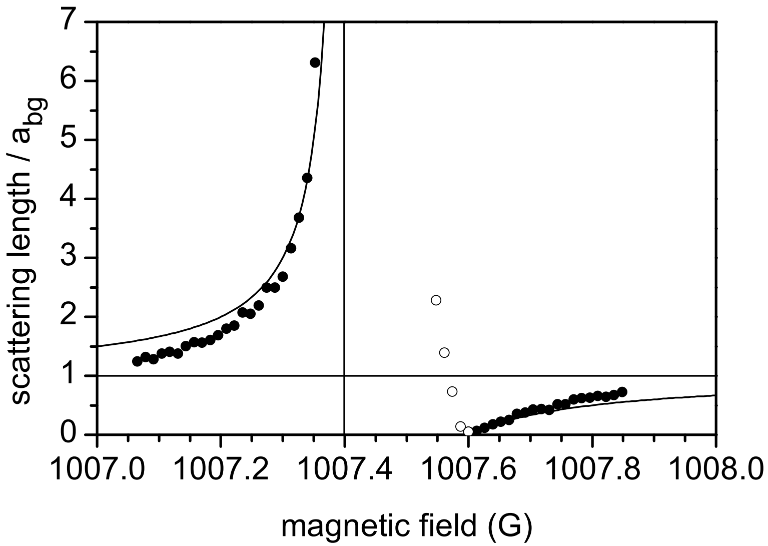
for cold atoms close to **Feshbach resonance**, possible to tune

- ❒ scattering length $\to \infty$
- ❒ effective range $\to 0$



Feshbach resonance in ^{87}Rb

O'Hara *et al.*, Science **298**, 2179 (2002)
Rempe *et al.*, PRA **68** 010702 (2003)
Regal *et al.*, Nature **424**, 47 (2003)
Bourdel *et al.*, PRL **91**, 020402 (2003)

expected: $a = a_{\text{bg}}\left(1 - \frac{\Delta B}{B - B_{\text{peak}}}\right)$

a_{bg} = "background" scattering length
ΔB = "width" of the Feshbach resonance

Quantum systems of particles with zero-range ('contact') interaction and their spectra

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Preliminary issue:

how to **construct models** that be

- mathematically unambiguous
- physically meaningful/realistic

Quantum systems of particles
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Hamiltonians are <u>not</u> ordinary Schrödinger operators:

$$H = \sum_{j=1}^{N} \left(\frac{\hbar^2}{2m_j}(-\Delta_{x_j}) + U_{\text{trap}}(x_j) \right) + \sum_{j<k}^{N} V(x_j - x_k)$$

$$H = \sum_{j=1}^{N} \left(\frac{\hbar^2}{2m_j}(-\Delta_{x_j}) + U_{\text{trap}}(x_j) \right) + \sum_{j<k}^{N} \left[\begin{array}{c} \text{interaction} \\ \text{only when } x_j = x_k \end{array} \right]$$

the zero-range interaction is modelled by boundary conditions dictated from physical heuristics at the coincidence hyperplanes

for low-energy (s-wave) two-body scattering, require:

$$-\frac{1}{r\Psi}\frac{\partial}{\partial r}(r\Psi) \xrightarrow{r\downarrow 0} \frac{1}{a} \qquad \text{i.e.,} \qquad \Psi \overset{r\downarrow 0}{\approx} \frac{e^{-r/a}}{r} \approx \left(\frac{1}{r}-\frac{1}{a}\right)$$

$\Psi \equiv \Psi(x_1,\dots,x_N)$, $r = |x_j - x_k|$,

$a =$ two-body scattering length in the channel (j,k)

In solving the equation for $l = 0$, one can therefore at small distances neglect the energy compared with the potential, so that the phase $= \frac{1}{ru}\frac{d(ru)}{dr}$ of the wave function will have a definite value α at distances small compared with the wave-length, but larger than a. Thus one can, instead of solving equation (3), work with the equation for free motion, but with the boundary condition that

$$-\frac{1}{ru}\frac{d(ru)}{dr} \to \alpha \qquad \text{for } r = 0.$$

The value of α can be deduced from the mass defect of H^2.

Bethe and Peierls, "*The quantum theory of diplon*", Proc. R. Soc. Lond. A 1935 **148**, 146-156 ("*diplon*" = nucleus of Deuterium ^{2}H, i.e., p-n)

$\Rightarrow$ **general idea:** the multi-particle Hamiltonian is basically the free Hamiltonian, except that it acts on wave-functions displaying the appropriate physical asymptotics in each two-body channel

notice: these are *particle-particle* boundary conditions of high-codimension; conceptually analogous to, but deeply different than, the b.c. in the modelling discussed in the talks by
$\rightarrow$ Exner,
$\rightarrow$ Stenzel,
$\rightarrow$ Holzmann,
$\rightarrow$ Stelzer,
and others, which are instead *one-particle* conditions relative to a *fixed locus* where the singular interaction is supported at (and with codim=1 or 2)

beside, those were implementation of 1dim Dirac $\delta^{(1)}$ distribution,
<u>no 3dim analogue here</u>: particle-particle contact interaction is NOT $\delta^{(3)}$

many approaches to define
multi-particle Hamiltonians with two-body **zero-range interaction**

① operator extensions (of free models away from coincidence)
(Berezin, Minlos, Faddeev, ...)
② nonstandard analysis
(Nelson, Alonso, Albeverio, Fenstad, Høegh-Krohn, ...)
③ Dirichlet forms
(Albeverio, Høegh-Krohn, Streit, ...)
④ approximation by finite range interactions + renormalisation
(Albeverio, Høegh-Krohn, Gesztesy, ...)
⑤ analysis of resolvents
(Grossmann, Høegh-Krohn, Mebkhout, ...)
⑥ quadratic forms
(Dell'Antonio, Figari, Teta, ...)

(here I mean: initiated by ... + epigones + new explorers)

today primarily ①, ④, ⑥

two general complications
affecting the definition of the model and its spectral analysis:

$$-\frac{1}{r\Psi}\frac{\partial}{\partial r}(r\Psi)\xrightarrow{r\downarrow 0}\frac{1}{a}$$

1) where/how to impose the Bethe-Peierls 'contact condition'?
• for *all* wave-functions in the Hamiltonian's operator/form domain?
• or just for eigenfunctions in the eigenvalue problem?
(second option customary in physics)
• impose it *point-wise* or in suitable *functional* sense?
($\rightarrow$ like for the 'radiation condition' in D. Mitrea's talk)

2) upon imposing the Bethe-Peierls 'contact condition',
is the resulting operator unambiguous? (i.e., self-adjoint)

Bethe-Peierls 'contact condition' $\stackrel{?}{\Rightarrow}$ H self-adjoint

two historical examples (paradigmatic, instructive):

- need of additional ('three-body') parameter in certain cases, in order to resolve the ambiguity ($\rightarrow$ Cacciapuoti's talk)

  Ter-Martirosyan, Skornyakov Sov. Phys. JETP (1956)
  Gribov, Sov. Phys. JETP (1960)
  Danilov, Sov. Phys. JETP (1961)
  Minlos, Faddeev, Sov. Phys. JETP (1962)

- BP-condition imposed for a too small domain yielded, for (2+1)-fermionic models, the wrong mass threshold for stability (lower semi-boundedness of the spectrum)

  Minlos, LNP (1987)
  Minlos, Mosc. Math. J. (2011,2012)
  Minlos, Uspekhi Mat. Nauk (2014)
  Correggi, Dell'Antonio, Finco, Michelangeli, Teta, MPAG (2015)
  Michelangeli, Ottolini, Rep. Math. Phys (2017,2018)

Observe: no need of additional three-body parameters for finite range interactions: ordinary U_{trap} and V give rise to essentially self-adjoint

$$H_{\text{finite range}} = \sum_{j=1}^{N} \Big(\frac{\hbar^2}{2m_j}(-\Delta_{x_j}) + U_{\text{trap}}(x_j) \Big) + \sum_{j<k}^{N} V(x_j - x_k)$$

and its spectral analysis is unambiguous. $H_{\text{zero range}}$, instead, might have multiple self-adjoint realisations.

Example (2 body): for $V \in L^{\frac{3}{2}}(\mathbb{R}^3) + L^{\infty}(\mathbb{R}^3)$,

(# negative EV's of $-\Delta + V$ w.r.t. $L^2(\mathbb{R}^3)$) $\leqslant C_{\text{LT}} \int_{\mathbb{R}^3} V_-^{3/2}(x)\,\mathrm{d}x$

Example (3 body): for $|V(x)| \lesssim \langle x \rangle^{-2}$, with $-\Delta + V \geqslant \mathbb{O}$ and zero-energy resonant

$H = \sum_{j=1}^{3}(-\Delta_{x_j}) + V(x_1 - x_2) + V(x_1 - x_3) + V(x_2 - x_3)$

(# negative EV's of H and $\leqslant -E$) $\sim C_0 \log E$ as $E \downarrow 0$

('**Efimov effect**')

Popular particle systems with zero-range interaction and with non-trivial spectral problems (many are open):

unitary Fermi gases

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'unitary limit', 'unitary regime':

- ❒ effective range $r_{\text{eff}} = 0$
- ❒ two-body scattering length $a = \infty$

i.e., limit of $\boldsymbol{k r_{\text{eff}} \ll 1}$, $\boldsymbol{k|a| \gg 1}$, $k := \sqrt{E}$

'**unitary**' because the two-body (low-energy) s-wave scattering amplitude

$$f_0(E) \;=\; \frac{e^{i\delta_0(E)}\sin\delta_0(E)}{\sqrt{E}} \;=\; -\frac{1}{\Big(\frac{1}{a} - \frac{r_{\text{eff}}}{2}E + \cdots\Big) + \mathrm{i}\sqrt{E}} \;\approx\; \frac{\mathrm{i}}{\sqrt{E}}$$

thus, f_0 reaches "*the max allowed by unitarity*";

recall indeed the Optical Theorem: $\mathfrak{Im}\, f_\ell(E) = \sqrt{E}\,|f_\ell(E)|^2$,

i.e., $f_\ell(E) = -\frac{1}{(\text{real function of } E) + \mathrm{i}\sqrt{E}}$

Popular particle systems with zero-range interaction
and with non-trivial spectral problems (many are open):

unitary Fermi gases

Notice:

- Bethe-Peierls contact condition 'at unitarity': $\frac{1}{r\Psi}\frac{\partial}{\partial r}(r\Psi) \xrightarrow{r\downarrow 0} 0$
- 'unitarity' is a typical 3-dim phenomenon
- 'unitarity' is essentially absent in higher order partial waves
- gases 'at unitarity' are an experimental fact (via Feshbach res.)
- typical interest in $N+M$ eteronuclear mixtures ($\rightarrow$ in 2 slides)

Popular particle systems with zero-range interaction
and with non-trivial spectral problems (many are open):

unitary Fermi gases

Universality:

❒ when $|a| \to \infty$ all details of the interaction are dropped out, no other parameters left to describe the interaction (challenging: no small parameters readily identifiable for perturbation theory)

❒ the only length (energy) units are $\dfrac{\hbar^2}{m}$ and L (size or the sample)

❒ scale invariance: the gas remains unitary if $L \mapsto \lambda L$,
with $E_k \mapsto \lambda^{-2} E_k$, $\Psi_k(x_1, \dots, x_N) \mapsto \lambda^{-3N/2} \Psi_k(x_1/\lambda, \dots, x_N/\lambda)$

Werner, Castin, "*Unitary gas in an isotropic harmonic trap*", Phys. Rev. A (2006)
Braaten, Hammer, "*Universality in few-body systems with large scatt. length*", Phys.Rep. (2006)
Giorgini, Pitaevskii, Stringari, "*Theory of ultra-cold atomic Fermi gases*", Rev. Mod. Phys. (2008)
Naidon, Endo, "*Efimov physics: a review*", Rep. Prog. Phys. (2017)

❒ typical interest in $N + M$ eteronuclear mixtures at unitarity

intriguing spectral challenges

➠ in the FEW-BODY PROBLEM

➠ in the MANY-BODY PROBLEM

(of course, as said, defining the model is an issue itself!)

2+1 fermionic system

Minlos, LNP (1987)
Minlos, Shermatov, Vestnik Moskov. Mat. Mekh. (1989)
Mogilner, Shermatov, Phys. Lett. A (1990)
Shermatov, Theor. Math. Phys. (2003)
Kartavtsev, Malykh, J. Phys. B (2007)
Endo, Naidon, Ueda, Few-Body Systems (2011)
Minlos, Mosc. Math. J. (2011,2012,2014)
Minlos, ISRN Math. Phys. (2012)
Finco, Teta, Rep. Math. Phys. (2012)
Correggi, Dell'Antonio, Finco, Michelangeli, Teta, Rev. Math. Phys. (2012)
Michelangeli, Schmidbauer, Phys. Rev. A (2013)
Minlos, Russian Math. Surveys (2014)
Correggi, Dell'Antonio, Finco, Michelangeli, Teta, MPAG (2015)
Yoshitomi, Math. Slovaca (2016)
Kartavtsev, Malykh, EPL (2016)
Michelangeli, Ottolini, Rep. Math. Phys. (2017,2018)
Moser, Seiringer, CMP (2017)
Becker, Michelangeli, Ottolini, MPAG (2018)

2+2 fermionic system

Michelangeli, Pfeiffer, J. Phys. A (2015)
Moser, Seiringer, MPAG (2018)

N+1 fermionic system

Minlos, SISSA ILAS (1994)
Minlos, Mosc. Math. J. (2011,2012)
Finco, Teta, Rep. Math. Phys. (2012)
Correggi, Dell'Antonio, Finco, Michelangeli, Teta, Rev. Math. Phys. (2012)
Correggi, Finco, Teta, EPL (2015)
Moser, Seiringer, CMP (2017)

and several other combinations
in formal treatments in the physical literature
(references above are mathematical)

For the **many-body** unitary Fermi gas,
a challenging (<u>and open</u>) spectral problem:

the Bertsch problem (George Bertsch, 1999)
(100$ prize...)

“*what are the ground state properties of the many-body system composed of spin-$\frac{1}{2}$ fermions interacting via a zero range, infinite scattering-length contact interaction?*”

(a problem originally intended as a challenge parameter-free model of **neutron matter** at subnuclear density $\rightarrow$ crust of neutron stars)

Baker, Phys.. Rev. C (1999)
Mihaila, Cardenas, SciTech Connect. (2008)
Iori, Macrì, Trombettoni, in *Mathematical Challenges of Zero-Range Interactions*, A. Michelangeli ed., Springer-INdAM (2021)

Explicitly: ground state energy per particle in a *free* Fermi gas

.
$$E_{\text{gs}}^{\text{free}}/N = \frac{3}{5}E_F$$

(N fermions occupying all states within the Fermi sphere),

where $E_F = \frac{\hbar^2}{2m}k_F^2 = \frac{\hbar^2}{2m}\left(\frac{3\pi^2 N}{V}\right)^{\frac{2}{3}}$.

Conjectured:

$$\lim_{N\to\infty}\frac{E_{\text{gs}}^{\text{unitary}}(N)}{N} = \xi\,\frac{3}{5}E_F\,, \qquad \xi = \text{'Bertsch parameter'}\,.$$

Mathematically ambiguity in modelling. Physical calculations in practice:

$$\lim_{N\to\infty}\ \lim_{\substack{a\to\infty\\ r_{\text{eff}}\to 0}}\frac{E_{\text{gs}}(a, r_{\text{eff}}, N)}{N} = \xi\,\frac{3}{5}E_F\,,$$

and order of limits affects the result.

$$\xi = \begin{cases} 0.41 & \text{Navon et al., Science (2010)} \\ 0.39 & \text{Luo, Thomas, J. Low Temp. Phys. (2009)} \\ 0.376 & \text{Ku et al., Science (2012)} \\ 0.37 & \text{Zürn et al., PRL (2013)} \\ 0.388 & \text{Schonenberg, Conduit, PRA (2017)} \end{cases}$$

The proof of the existence of the dimensionless Bertsch **spectral parameter** ξ in some rigorous and meaningful limit, and its calculation, has become a theoretical challenge.

With $0 < \xi \leqslant 1$ the ground state $E_{\rm gs}^{\rm unitary}$ would be that of a very unusual gas, a super-fluid with a pairing gap of the order of the Fermi energy, the largest pairing gap in any physical system, in addition to its universal properties largely independent of the details of the interaction.

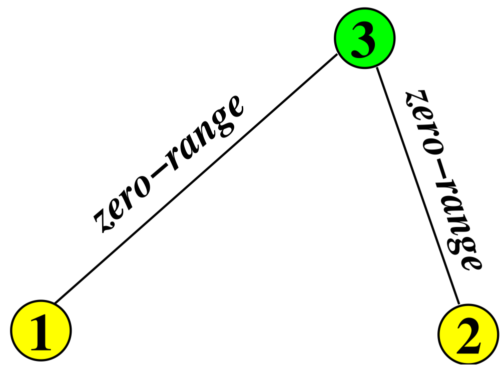
To be stressed: a hard problem mathematically!

➠ rigorous construction of N-body Hamiltonian at unitarity unknown for $N \geqslant 4$

➠ let alone the limit $N \to \infty$

➠ uncontrolled limit $r_{\rm eff} \to 0$, at fixed $N \geqslant 3$ (known for $N = 2$)

More on 2+1 fermionic system.



Two identical fermions of mass 1,
zero-range interaction with a third particle of mass m.

Preparations:

❒ $\boldsymbol{\mu} := \frac{2}{m+1}$, $\boldsymbol{\nu} := \frac{m(m+2)}{(m+1)^2} = 1 - \frac{\mu^2}{4}$

❒ $$\widehat{(T_\lambda\,\xi)}(p) := 2\pi^2\sqrt{\nu p^2 + \lambda}\,\widehat{\xi}(p) + \int_{\mathbb{R}^3} \frac{\widehat{\xi}(q)}{p^2 + q^2 + \mu p\cdot q + \lambda}\,\mathrm{d}q\,, \qquad p \in \mathbb{R}^3$$

for fixed $\lambda > 0$ ('charge operator').
Maps continuously $H^s(\mathbb{R}^3)$ into $H^{s-1}(\mathbb{R}^3)$ for any $s \in (-\frac{1}{2}, \frac{3}{2})$.

❒ $$\widehat{u_\xi^\lambda}(p_1, p_2) := \frac{\widehat{\xi}(p_1) - \widehat{\xi}(p_2)}{p_1^2 + p_2^2 + \mu\, p_1\cdot p_2 + \lambda}\,, \quad \xi \in H^{-\frac{1}{2}}(\mathbb{R}^3) \equiv \text{'space of charges'}$$

❒ $$\Lambda(m) := \frac{2}{\pi}(m+1)^2\Big(\frac{1}{\sqrt{m(m+2)}} - \arcsin\frac{1}{m+1}\Big)$$

('Efimov trascendental function') monotone decreas. $\mathbb{R}^+ \to \mathbb{R}^+$ bijection

❒ $m^* \approx (13.607)^{-1}$, the unique root of $\Lambda(m) = 1$.

The Hamiltonian H_α: for $\underline{\alpha \in \mathbb{R}}$ and $\underline{m > m^*}$ define

$$\mathcal{D}(H_\alpha) \;:=\; \left\{ g = F^\lambda + u_\xi^\lambda \;\middle|\; \begin{array}{c} F^\lambda \in H^2_{\mathsf{f}}(\mathbb{R}^3 \times \mathbb{R}^3)\,, \\ \xi \in H^{\frac{1}{2}}(\mathbb{R}^3)\,,\; (T_\lambda + \alpha \mathbb{1})\xi \in H^{\frac{1}{2}}(\mathbb{R}^3)\,, \\ \text{plus the boundary conditions } (\textbf{tms}') \end{array} \right\}$$

$$(\textbf{tms}') \qquad \int_{\mathbb{R}^3} \widehat{F^\lambda}(p_1,p_2)\,\mathrm{d}p_2 \;=\; \Big((T_\lambda + \alpha)\,\xi\Big)^{\widehat{}}\,(p_1)\,,$$

$$(H_\alpha + \lambda \mathbb{1})\, g \;:=\; (H_{\mathrm{free}} + \lambda \mathbb{1})\, F^\lambda$$

$$=\; \Big(-\Delta_{x_1} - \Delta_{x_2} - \tfrac{2}{m+1} \nabla_{x_1} \cdot \nabla_{x_2} + \lambda \Big)\, F^\lambda\,.$$

acting on $\mathcal{H} = L^2_{\mathsf{f}}(\mathbb{R}^3 \times \mathbb{R}^3, \mathrm{d}x_1 \mathrm{d}x_2)$
(three-body Hilbert space in internal coordinates, c.m. factored out)

Theorem. Let $m > m^*$.

(1) H_α is self-adjoint on $\mathcal{H}$, and

$$\begin{aligned} \inf\sigma(H_\alpha) &= 0 && \text{if } \alpha \geqslant 0 \\ \inf\sigma(H_\alpha) &\geqslant -\tfrac{\alpha^2}{4\pi^4(1-\Lambda(m)^2)} && \text{if } \alpha < 0\,. \end{aligned}$$

(2) H_α is an extension of

$$\begin{aligned} \mathring{H} &:= -\Delta_{x_1} - \Delta_{x_2} - \tfrac{2}{m+1}\nabla_{x_1}\cdot\nabla_{x_2} \\ \mathcal{D}(\mathring{H}) &:= C_0^\infty((\mathbb{R}^3\times\mathbb{R}^3)\setminus(\Gamma_1\cup\Gamma_2))\cap\mathcal{H} \end{aligned}$$

($\Gamma_1 := \{x_1 = 0\}$, $\Gamma_2 := \{x_2 = 0\}$, the coincidence hyperplanes)

(3) every $g \in \mathcal{D}(H_\alpha)$ satisfies

$$\int_{\substack{p_2\in\mathbb{R}^3 \\ |p_2|<R}} \widehat{g}(p_1,p_2)\,\mathrm{d}p_2 \overset{R\to+\infty}{=} (4\pi R+\alpha)\,\widehat{\xi}(p_1) + o(1) \qquad \textbf{(tms)}$$

the Ter-Martirosyan–Skornyakov condition (**(tms)** $\Leftrightarrow$ **(tms$'$)**)

(4) equivalently, with $\boldsymbol{a} := -(4\pi\alpha)^{-1}$

$$g_{\mathrm{av}}(x_1;|x_2|) := \frac{1}{4\pi}\int_{\mathbb{S}^2} g(x_1,|x_2|\Omega)\mathrm{d}\Omega \overset{|x_2|\to 0}{=} c_g\left(\frac{1}{|x_2|} - \frac{1}{a}\right)\xi(x_1) + o(1)$$

the Bete-Peierls contact condition

- Rigorously established in

  Correggi, Dell'Antonio, Finco, Michelangeli, Teta, Rev. Math. Phys. (2012)

  Michelangeli, Schmidbauer, Phys. Rev. A (2013)

  Michelangeli, Ottolini, Rep. Math. Phys. (2017,2018)

  Becker, Michelangeli, Ottolini, MPAG (2018)

  Michelangeli, Rev. Math. Phys. (2021)

both by extension techniques and by quadratic form methods.
Previous attempts: formal / heuristic / numerical / (or wrong).

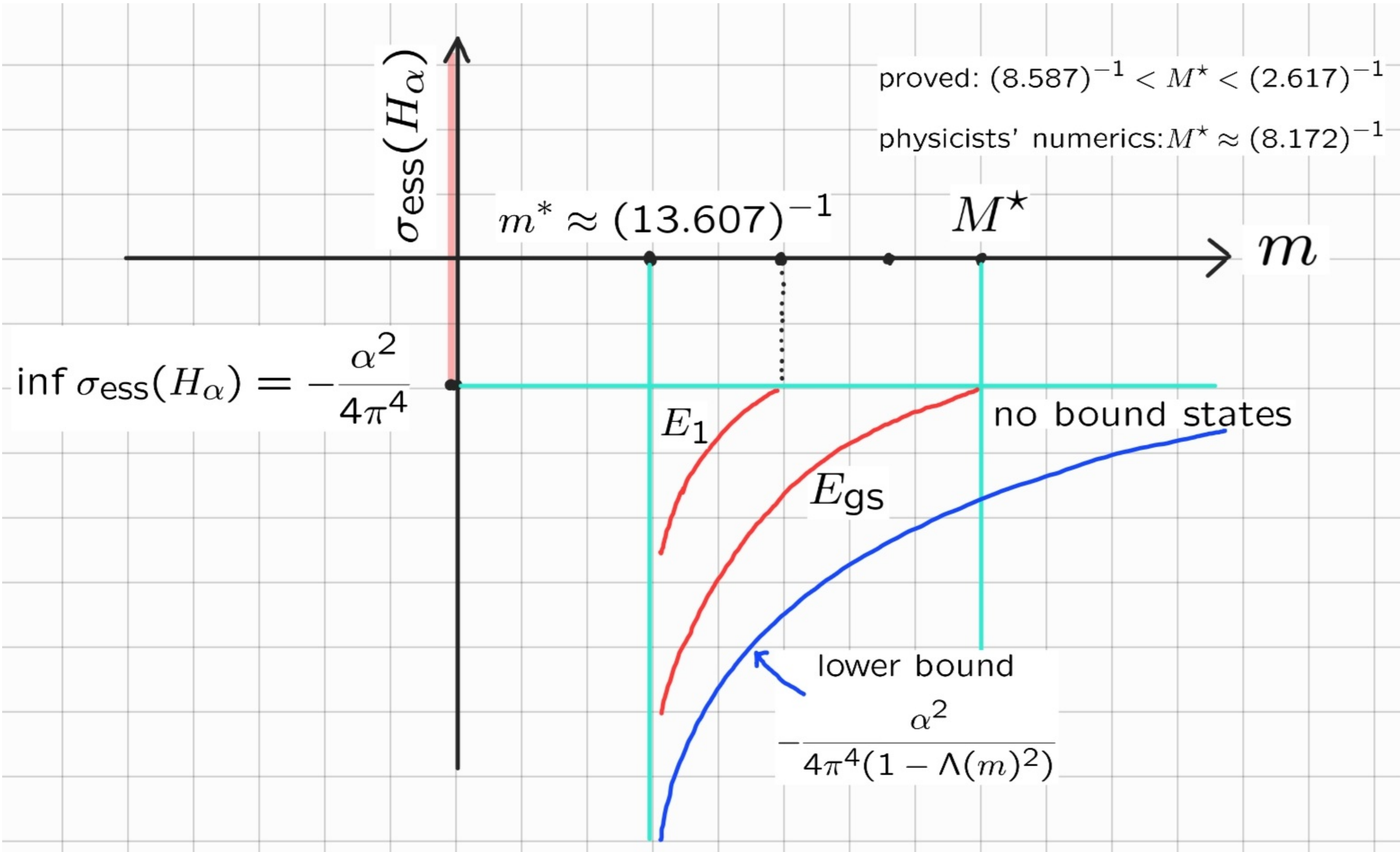
- Model of non-trivial contact interaction supported Γ_1 and Γ_2.

- Each two-body channels exhibits
  precisely the physical behaviour $\Psi \sim (\frac{1}{r} - \frac{1}{a})$ as $r \downarrow 0$.

- α is the inverse scattering length (two-body parameter)

Theorem. Michelangeli, Schmidbauer, Phys. Rev. A (2013)
Becker, Michelangeli, Ottolini, MPAG (2018)
Michelangeli, Rev. Math. Phys. (2021)

$(\alpha < 0)$



Based on the following key fact:

eigenfunctions Ψ_E at $-E<0$: $\widehat{\Psi_E}=\widehat{u_\xi^E}=\frac{\widehat{\xi}(p_1)-\widehat{\xi}(p_2)}{p_1^2+p_2^2+\mu\, p_1\cdot p_2+E}$

for suitable ξ of angular symmetry $\ell=1$

satisfying $T_E\xi+\alpha\xi=0$ (the 'Ter-Martirosyan Skornyakov equation')

+ study of the (non-local) integro-differential operator T_E

Open (work in progress):

- ❒ rigorous derivation of threshold $M^\star$
- ❒ mass threshold for EV's to disappear/embed in $\sigma_{\text{cont}}(H_\alpha)$
- ❒ spectral behaviour as $m\downarrow m^*$
- ❒ rigorize physicist's formal (yet efficient!) arguments

❒ additional multiplicity of models for $m\in(0,m^{**})$, $m^{**}\approx(8.62)^{-1}$
(each one characterised by an extra three-body parameter)

❒ counterpart problem for bosons