On the large-distance asymptotics of the ground state of the Schrödinger-Newton, a.k.a. Choquard equation

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Outline

We will talk about the nonlinear Schrödinger equation

$$-\Delta\psi(\mathbf{s}) - 2\int_{\mathbb{R}^3} \frac{1}{|\mathbf{s}-\mathbf{s}'|}|\psi|^2(\mathbf{s}')d^3s'\,\psi(\mathbf{s}) = E\psi(\mathbf{s}) \tag{1}$$

where $\mathbf{s} = (x,y,z) \in \mathbb{R}^3$ and $\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ is the Laplacian.

We inquire into the unique (modulo translations) positive solution $\psi_1 : \mathbb{R}^3 \to \mathbb{R}_+$ satisfying $\int |\psi_1|^2(\mathbf{s})d^3s = 1$, and into its eigenvalue E_1.

The integro-PDE formulation of the problem is equiv. to the PDE system

$$-\Delta u(\mathbf{s}) + V(\mathbf{s})u(\mathbf{s}) = -u(\mathbf{s}), \tag{2}$$

$$\Delta V(\mathbf{s}) = |u|^2(\mathbf{s}); \tag{3}$$

together with $u > 0$ and $\int |u|^2(\mathbf{s})d^3s < \infty$, and $V(\mathbf{s}) \to 0$ as $|\mathbf{s}| \to \infty$.

N.B.:

$$\int |u|^2(\mathbf{s})d^3s = 8\pi/\sqrt{|E|}\,.$$

By uniqueness, $\psi_1(\mathbf{s}) = \psi_1(r)$, where $r = |\mathbf{s}| \implies$ (2)+(3)$\equiv 4^{th}$ order ODE.

Different physical models all end up with the same equation!
(mathematically speaking)

1) Condensed matter: the polaron (L. **Landau**; S. **Pekar**; H. **Fröhlich**)
2) Condensed matter: 1-component quantum plasma (P. **Choquard**)
3) Dark matter: gravitating spin-0 bosons (J. **Rueda** & R. **Ruffini**)
4) Foundations of QM: gravity-induced collapse of WF (R. **Penrose**)

N.B.:

E. H. Lieb coined the name **Choquard's equation** for (1)
Other authors have called it **Pekar's equation**.
R. Penrose called (1) the **Schrödinger–Newton** eqn.
D. Greiner & G. Wunner called (1) the **Newton–Schrödinger** eqn.
Yet other authors called (2),(3) the **Schrödinger–Poisson system**.

BUT: The first who could have written it down is ... Erwin Schrödinger:
0) Foundations of QM: interpretation of Ψ as matter wave.

A selective list of important rigorous papers on the ground state:

E. H. Lieb, Studies Appl. Math (1977).

M. D. Donsker and S. R. S. Varadhan, Phys. Rep. (1981).

M. D. Donsker and S. R. S. Varadhan, CPAM (1983).

E. H. Lieb and L. E. Thomas, CMP (1997).

K. P. Tod and I. Moroz, Nonlinearity (1999).

K. P. Tod, Phys. Lett. A (2001).

V. Moroz and J. van Schaftingen, J. Funct. Anal. (2013).

A recent survey of rigorous results for equation (1), resp. (2),(3), is:

V. Moroz and J. van Schaftingen, J. Fixed Pt. Theor. Appl. (2017).

The asymptotic limit of the CPSN... equation

Assuming for the moment that $|\psi|^2(r)$ is exponentially small (in r) for large r, the CPSN... equation (1) takes on the asymptotic form

$$-\Delta\psi^{(\infty)}(\mathbf{s}) - 2\frac{1}{|\mathbf{s}|}\psi^{(\infty)}(\mathbf{s}) = E\psi^{(\infty)}(\mathbf{s}) \tag{4}$$

which is formally a Schrödinger equation for a "hydrogenic ion." The pertinent normalized ground state solution of (4) (assuming (4) holds everywhere) indeed is exponentially decaying,

$$\psi_1^{(\infty)}(r) = A\exp(-r)$$

with ground state energy

$$E_1^{(\infty)} = -1.$$

Mixed messages

- K. P. Tod and I. Moroz (1999) claim, without proof, that if $u(r)$ is a positive radial solution to (2),(3), then

$$u(r) = Ae^{-r}/r + \ l.o.t.$$

- D. Kumar and V. Soni (2000) claim that

$$u(r) = Ae^{-r} + \ l.o.t.$$

  Based on this claim they concluded that the ground state energy $E_1 = -1$.
- K. P. Tod (2001) proves that $E_1 > -1$.
- V. Moroz and J. van Schaftingen (2013) prove that

$$u(r) = Ae^{-r}/r^{1-\|u\|_2^2/8\pi} + \ l.o.t.$$

  where $\|u\|_2$ is the L^2 norm of u.

Remarks on the conflicting results

- K. P. Tod and I. Moroz announced their claim in a joint paper with R. Penrose (1998).
- Their claim was repeated in the Ph.D. thesis of R. Harrison (2001).
- What *IS* proved by Tod and I. Moroz is that for every positive $C < 1$ there are $A > 0$ and $b > 0$ such that $u(r) < Ae^{-Cr}/r$ for all $r > b$, (incidentally, a factor e^{Cb} is obviously missing at r.h.s.(3.9) of their paper); however, such an upper bound alone cannot establish the asymptotic behavior claimed.
- Kumar and Soni conclude from their asymptotics of $u(r)$ that $E_1 = -1$; however, a nonlocal quantity like an eigenvalue cannot be determined by a truncated asymptotic expansion!
- The value of $\|u\|_2^2$ was left open by V. Moroz and van Schaftingen. Their result rules out the asymptotic behavior claimed by Tod and I. Moroz, but leaves the possibility that Kumar and Soni are right.

QUESTION: What is the value of $\|u\|_2^2$?

We know that $\|u\|_2^2 > 0$, but is:

- $\|u\|_2^2 \in (0, 8\pi)$? If so, $r^{\|u\|_2^2/8\pi - 1}$ is **decreasing.**
- $\|u\|_2^2 = 8\pi$? If so, $r^{\|u\|_2^2/8\pi - 1} = 1$ is **constant** (Kumar-Soni).
- $\|u\|_2^2 \in (8\pi, 16\pi)$? If so, $r^{\|u\|_2^2/8\pi - 1}$ is **increasing** and **concave.**
- $\|u\|_2^2 = 16\pi$? If so, $r^{\|u\|_2^2/8\pi - 1} = r$ is **increasing** and **linear.**
- $\|u\|_2^2 > 16\pi$? If so, $r^{\|u\|_2^2/8\pi - 1}$ is **increasing** and **convex.**

We will prove (in parts assisted by MAPLE [for convenience]):

Proposition: *The L^2 norm of the positive H^1 solution $u(r)$ of (2),(3) obeys the bounds*

$$2^{1/3}3\pi^2 \leq \|u\|_2^2 \leq 8\pi^{3/2}. \tag{5}$$

Numerically,

$$11.875\pi \leq \|u\|_2^2 \leq 14.18\pi. \tag{6}$$

COMMENTS: This is strong enough to rigorously rule out the asymptotic form of $u(r)$ proposed by Kumar and Soni (since $2^{1/3}3\pi^2 > 8\pi$), showing that the monomial prefactor of e^{-r} is increasing with r, and strong enough (since $8\pi^{3/2} < 16\pi$), to prove that the monomial prefactor of e^{-r} is strictly concave.

Proof of the Proposition

For convenience, here is (1) again,

$$-\Delta\psi(\mathbf{s}) - 2\int_{\mathbb{R}^3} \frac{1}{|\mathbf{s}-\mathbf{s}'|}|\psi|^2(\mathbf{s}')d^3s'\,\psi(\mathbf{s}) = E\psi(\mathbf{s}). \tag{7}$$

N.B.: In this form the Schrödinger–Newton equation appears in Lieb's work (1977; Choquard's eqn.), and in a paper by Greiner and Wunner (2006; Newton–Schrödinger eqn.).
Eq.(7) is the Euler–Lagrange equation for minimizing the functional

$$\mathcal{E}(\psi) := \int_{\mathbb{R}^3}|\nabla\psi|^2(\mathbf{s})d^3s - \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\frac{|\psi|^2(\mathbf{s})|\psi|^2(\mathbf{s}')}{|\mathbf{s}-\mathbf{s}'|}d^3sd^3s' \tag{8}$$

on the Sobolev space $H^1(\mathbb{R}^3)$ under the constraint $\int_{\mathbb{R}^3}|\psi|^2(\mathbf{s})d^3s = 1$.
The eigenvalue E is the Lagrange multiplier for this constraint.

Proof of the Proposition (cont.^{d})

Let $\psi_1(r)$ be the minimizer.
For real $\lambda > 0$, define $\psi_\lambda(r) := \lambda^{3/2}\psi_1(\lambda r)$. Then $\forall\,\lambda:\ \|\psi_\lambda\|_2 = 1$.
By noting that $\frac{d}{d\lambda}\mathcal{E}(\psi_\lambda)|_{\lambda=1} = 0$ we obtain the **virial identity**

$$2\int_{\mathbb{R}^3}|\nabla\psi_1|^2(\mathbf{s})d^3s = \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\frac{|\psi_1|^2(\mathbf{s})|\psi_1|^2(\mathbf{s}')}{|\mathbf{s}-\mathbf{s}'|}d^3sd^3s'. \tag{9}$$

On the other hand, setting $\psi = \psi_1$ in (7), then multiplying (7) by ψ_1 and integrating over $\mathbb{R}^3$, yields for the ground state energy

$$E_1 = \int_{\mathbb{R}^3}|\nabla\psi_1|^2(\mathbf{s})d^3s - 2\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\frac{|\psi_1|^2(\mathbf{s})|\psi_1|^2(\mathbf{s}')}{|\mathbf{s}-\mathbf{s}'|}d^3sd^3s'. \tag{10}$$

Now using (9) in (10) and also in (8), by comparison we obtain

$$E_1 = 3\,\mathcal{E}(\psi_1). \tag{11}$$

Thus, upper or lower bounds on $\mathcal{E}(\psi)$ over H^1 under the normalization constraint $\|\psi\|_2 = 1$ translate into corresponding upper and lower bounds on the ground state energy E_1.

Proof of the Proposition (cont.^{d})

Next, by Sobolev's inequality [cf. p.174 in Tod (2001)],

$$\int_{\mathbb{R}^3} |\nabla\psi|^2(\mathbf{s}) d^3s \geq 3\left[\frac{\pi}{2}\right]^{\frac{4}{3}} \left(\int_{\mathbb{R}^3} |\psi|^6(\mathbf{s}) d^3s\right)^{\frac{1}{3}}. \tag{12}$$

On the other hand, the Hardy–Littlewood–Sobolev inequality yields

$$\int_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|\psi|^2(\mathbf{s})|\psi|^2(\mathbf{s}')}{|\mathbf{s}-\mathbf{s}'|} d^3s d^3s' \leq \frac{4}{3}\left[\frac{8}{\pi}\right]^{\frac{1}{3}} \left(\int_{\mathbb{R}^3} |\psi|^{\frac{12}{5}}(\mathbf{s}) d^3s\right)^{\frac{5}{3}}, \tag{13}$$

and Hölder's inequality gives [cf. p.175 in Tod (2001)]

$$\int_{\mathbb{R}^3} |\psi|^{\frac{12}{5}}(\mathbf{s}) d^3s \leq \left(\int_{\mathbb{R}^3} |\psi|^2(\mathbf{s}) d^3s\right)^{\frac{9}{10}} \left(\int_{\mathbb{R}^3} |\psi|^6(\mathbf{s}) d^3s\right)^{\frac{1}{10}}, \tag{14}$$

which simplifies because $\int_{\mathbb{R}^3} |\psi|^2(\mathbf{s}) d^3s = 1$.

Proof of the Proposition (cont.^{d})

Now setting $\int_{\mathbb{R}^3} |\psi_1|^6(\mathbf{s})d^3s =: x^6$, our chain of inequalities yields

$$\mathcal{E}(\psi_1) \geq 3\left[\frac{\pi}{2}\right]^{\frac{4}{3}} x^2 - \frac{4}{3}\left[\frac{8}{\pi}\right]^{\frac{1}{3}} x; \tag{15}$$

and since we don't know x, to be on the safe side we minimize r.h.s.(15) w.r.t. $x > 0$ and obtain

$$\mathcal{E}(\psi_1) \geq -\frac{32}{27}\frac{2^{1/3}}{\pi^2} \approx -0.1513. \tag{16}$$

Multiplication by 3 yields

$$E_1 \geq -\frac{32}{9}\frac{2^{1/3}}{\pi^2} \approx -0.4539. \tag{17}$$

Proof of the Proposition (cont.^{d})

Rescaling the ground state energy to $E = -1$ yields $\|u\|_2^2 = 8\pi/\sqrt{|E_1|}$, and so, since also $E_1 < 0$, by (17) we have

$$\|u\|_2^2 \geq 2^{1/3} 3\pi^2 \approx 11.875\pi \tag{18}$$

This proves the lower bound l.h.s.(5) in our Proposition.
To obtain the upper bound in our Proposition we insert the Gaussian trial wave function $\psi_G(r) := \exp(-r^2/2R^2)/(\pi^{3/4}R^{3/2})$ into $\mathcal{E}(\psi)$ and minimize w.r.t. R, obtaining an upper bound on $\mathcal{E}(\psi_1)$. Rescaling to units in which the ground state energy $E = -1$ yields r.h.s.(5). □

REMARKS: Our upper and lower bounds on E_1 are slightly strikter than corresponding bounds obtained by K. P. Tod (2001), who did not extract upper and lower bounds on $\|u\|_2^2$ from his bounds.
Our upper bound was computed algebraically with the help of MAPLE.

Comments on the MAPLE computations

- $\mathcal{E}(\psi)$ is a sum of a three- and a six-dimensional integral, but ...
- ψ_1 is invariant under $SO(3)$ action, so for $\psi = \psi(r)$, ...
- $\mathcal{E}(\psi)$ can be rewritten as

$$\mathcal{E}(\psi) = 4\pi \int_0^\infty |\psi'(r)|^2 r^2 dr - 4\pi \int_0^\infty r^2 \psi(r)^2 \left(\int_r^\infty \frac{M(s)}{s^2} ds \right) dr$$

where

$$M(r) = 4\pi \int_0^r |\psi(s)|^2 s^2 ds.$$

N.B.: $$\lim_{r\to\infty} M(r) = 1.$$

Comments on the MAPLE computations cont.[d]

- Paul Tod uses

$$\psi_T(r) = \frac{1}{\sqrt{\pi R^3}} \exp\left(-\frac{r}{R}\right)$$

which yields

$$3\mathcal{E}(\psi_T) = \frac{1}{R^2} - \frac{5}{8R} \geq -\frac{75}{256} \approx -0.293 \geq E_1$$

N.B.: Multiplication by $\frac{1}{2}\frac{G^2 m^5}{\hbar^2}$ gives Penrose's quantum units.

- Using instead a Gaussian,

$$\psi_G(r) = \frac{1}{\sqrt{\sqrt{\pi}^3 R^3}} \exp\left(-\frac{1}{2}\frac{r^2}{R^2}\right)$$

yields

$$3\mathcal{E}(\psi_G) = \frac{3}{2R^2} - \frac{\sqrt{2}}{\sqrt{\pi}\, R} \geq -\frac{1}{\pi} \approx -0.31831 \geq E_1$$

Prologue

Although numerical studies of the Schrödinger–Newton equation have been carried out by I. Moroz, R. Penrose, and Tod (1998); by R. Harrison (2001); by Greiner and Wunner (2006); and by a few other authors cited in those papers, we are unaware of any which has addressed itself to the power of the radial monomial correction factor to the exponential function.

Yet information about $\|u\|_2^2$ can be extracted from numerical data in the paper of Greiner and Wunner (2006), by rescaling, revealing that $\|u\|_2^2 \approx 14.04\pi$.

We have carried out our own numerical study and directly computed that $\|u\|_2^2 \approx 14.03\pi$, compatible with the result extracted from the paper of Greiner and Wunner (2006) by rescaling.

Thus the monomial prefactor of e^{-r} is $\propto r^\beta$ with $\beta \approx 0.754$, i.e. increasing and strictly concave.

COMMENTS

We converted the Schrödinger-Newton eq. into a 4th order ODE

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\left(\frac{1}{u(r)}\frac{1}{r^2}\left(\frac{d}{dr}\left(r^2\frac{d}{dr}u(r)\right)\right)\right)\right) = u^2(r).$$

Data: $u'(0) = 0 = u'''(0)$; while $u(0) > 0$ and $u''(0) < 0$ to be found! Our numerical computations were carried out with MAPLE's Cash–Karp fourth-fifth order Runge–Kutta method with degree four interpolant (ck45), which proved more suitable than MAPLE's default Runge–Kutta–Fehlberg routine rkf45. To overcome the enormous variations over the range of $u(r)$ we solved the ODE for $\ln u(r)$ and asked for 70 digits precision during the computation. The interval halving iterations to determine the correct initial data $u(0)$ and $u''(0)$ to yield energy $E = -1$ were terminated after a precision of three significant digits had been achieved, though.

Fig. 1: Sequence of approximates to u_∞ versus r.

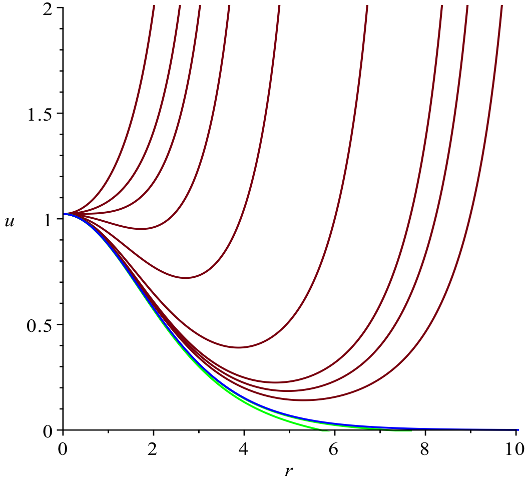

Figure: 1. Shown are successive approximations to the gound state solution $u(r)$ of (2),(3). The ground state is the lower envelope to the red curves, and the upper envelope to the green curves.

Fig. 2: The ground state $u(r)$

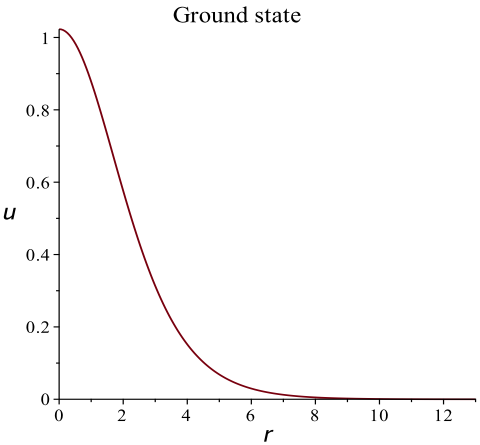

Figure: 2. Numerical approximation to the gound state solution $u(r)$ of (2),(3).

Fig. 3: The mass function $M(r) := 4\pi \int_0^r |u(s)|^2 s^2 ds$.

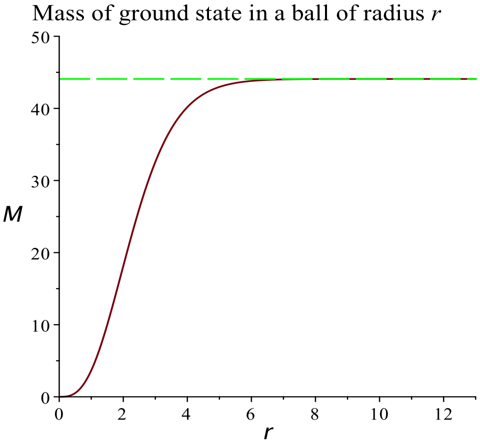

Figure: 3. Shown is $M(r) := 4\pi \int_0^r |u(s)|^2 s^2 ds$ for the gound state solution $u(r)$ of (2),(3); the horizontal asymptote is at $14.03\pi \approx \|u\|_2^2 = \lim_{r\to\infty} M(r)$.

Fig. 4: The natural logarithm of $u(r)$.

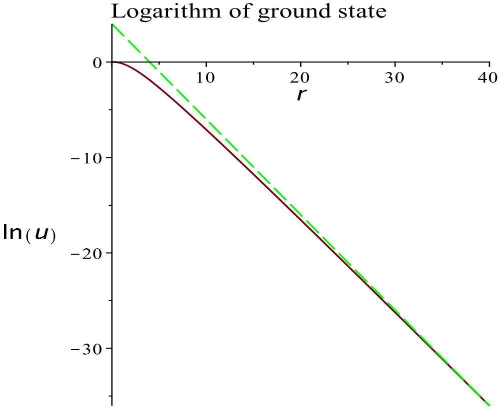

Figure: 4. Shown is the natural logarithm of the gound state solution $u(r)$ of (2),(3), together with a straight line of slope -1. Apparently the figure suggests a purely exponential decay of the ground state $u(r)$, but appearances are misleading, as visualized in Fig. 5.

Fig. 5: Zooming in: $\mathrm{Id}(r) + \ln u(r)$.

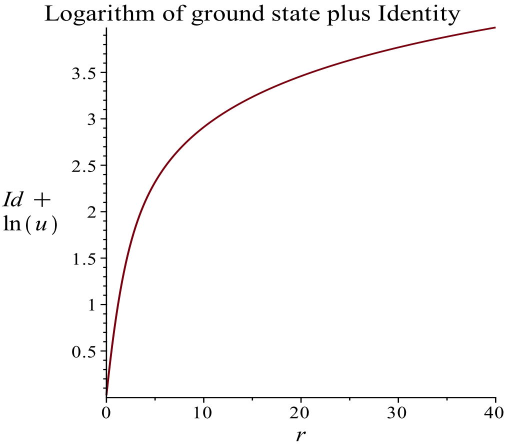

Figure: 5. Shown is $r + \ln u(r)$ versus r for the gound state solution $u(r)$ of (2),(3). Fig. 5 reveals that the map $r \mapsto r + \ln u(r)$ is not asymptotic, for large r, to a constant function, which it would be if $u(r) \sim A\exp(-r)$.

Fig. 6: Natural logarithm of u_∞/u versus r.

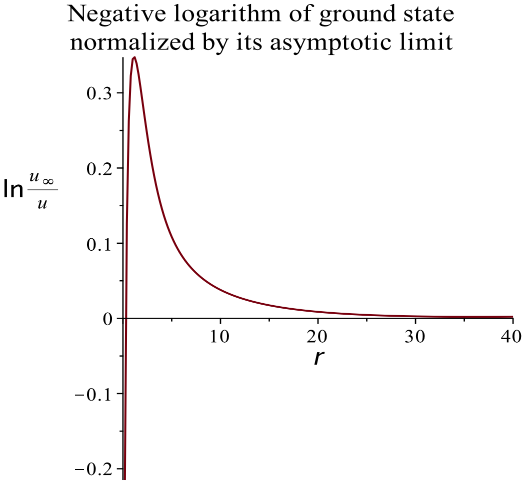

Figure: 6. Shown is the negative natural logarithm of the ratio of the gound state solution $u(r)$ of (2),(3) over its asymptotic limit $u_\infty(r) = Ar^\beta \exp(-r)$ with $\beta \approx 0.754$ and $A \approx 3.37$.

TEST

As a test for our results we rescaled the ground state energy $E = E_1$ for (7), computed numerically in Greiner-Wunner (2006) to be $E_1 = -0.325(74)$, into our units in which the ground state energy $E = -1$. This yields $\|u\|_2^2 = 8\pi/\sqrt{|E_1|} \approx 44.09$, in good agreement with our result $14.03\pi \approx 44.08$.

Andrey Yudin's observation (personal communication)

Recall: The hydrogenic Schrödinger equation (4) is the asymptotic form of the SN equation (1).
Rescaling (4) into the variables of the system (2), (3) yields

$$-\Delta u(\mathbf{s}) - \frac{\|u\|^2}{4\pi}\frac{1}{|\mathbf{s}|}u(\mathbf{s}) = -u(\mathbf{s}). \tag{19}$$

Knowing the leading order asymptotics, with $\|u\|^2$ treated as a positive parameter, MAPLE tells you that (19) is solved by

$$u(\mathbf{s}) = A \times U(1 - \|u\|^2/8\pi, 2, 2r) \times \exp(-r), \tag{20}$$

where $A > 0$ is an amplitude to be determined from the numerical solution, as is $\|u\|^2$, while $U(a, b, z)$ is Kummer's U-function; the unique solution to the confluent hypergeometric equation having asymptotics $u(z) \sim z^{-a}$ for $\Re z > 0$ (and $\arg(z)$ near zero).

Yudin's proposal may hit the nail on the head!

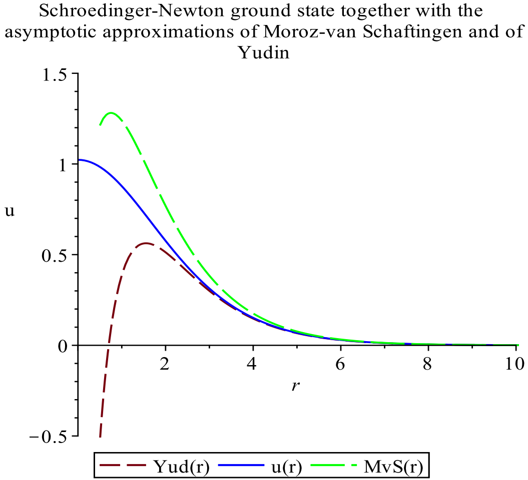

Figure: 7. The numerically computed gound state solution $u(r)$ of (2),(3) together with its asymptotic limit $u_\infty(r) = Ar^\beta \exp(-r)$ with $\beta \approx 0.754$ and $A \approx 3.37$, and with Yudin's extended asymptotic function.

Open Questions concerning the Ground State!

- Can one prove that the Kummer function U captures all asymptotic expansion factors of $\exp(-r)$ which are of power-law type? Does it miss only those which are themselves "small beyond all orders"?
- There surely will be correction terms to the (negative) power series expansion of the prefactor of $\exp(-r)$ showing up if one expands beyond all orders. What are these "transseries"?

$\longrightarrow$ Joint projects with Andrey Yudin and Ovidiu Costin.

Radially symmetric excited states

P.-L. Lions (1980) proved that there are infinitely many oscillatory radial solutions to (1), associated with discrete eigenvalues E_n, $n \in \mathbb{N}$. Various authors computed them numerically; in particular Greiner & Wunner (2006), who give a plausible vindication of applying the semi-classical **Einstein-Brillouin-Keller** quantization, which predicts

$$E_n = -\frac{1}{(n - \mu_n)^2} \tag{21}$$

where the μ_n are so-called quantum defects. Greiner-Wunner extract from their numerical computations the empirical rule

$$\mu_n \approx -1.729 - 1.291n. \tag{22}$$

Inserted into the EBK formula this gives the empirical spectral rule:

$$E_n \approx -0.191 \frac{1}{(n + 0.754)^2}. \tag{23}$$

Can one prove this? Note that $u(r) \sim A\, r^{0.754}\, e^{-r}$ — coincidence?

THANK YOU FOR YOUR ATTENTION!

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Slightly weaker results than reported here appeared in:

M.K.-H. Kiessling,
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Phys. Lett. A. **395**:127209 (2021); "errata" in preparation.