On the asymptotic decay of the Schrödinger–Newton ground state

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The asymptotics of the ground state $u(r)$ of the Schrödinger–Newton equation in $\mathbb{R}^3$ was determined by V. Moroz and J. van Schaftingen to be $u(r) \sim Ae^{-r}/r^{1-\|u\|_2^2/8\pi}$ for some $A > 0$, in units in which the ground state energy is $-1$. They left open the value of $\|u\|_2^2$, the squared $L^2$ norm of $u$. Here it is rigorously shown that $2^{1/3}3\pi^2 \leq \|u\|_2^2 \leq 8\pi^{3/2}$. It is reported that numerically $\|u\|_2^2 \approx 14.03\pi$, revealing that the monomial prefactor of $e^{-r}$ increases with $r$ in a concave manner. Asymptotic results are proposed for the Schrödinger–Newton equation with external $-K/r$ potential, and for the related Hartree equation of a bosonic atom or ion.

I. INTRODUCTION

The non-linear integro-differential equation

$$-\Delta u(s) + u(s) = \frac{1}{4\pi} \int_{\mathbb{R}^3} \frac{1}{|s-s'|} |u^2(s')d^3s' u(s)$$

(1)

shows up in a variety of models in physics, and as such is variously known as Pekar’s equation, Choquard’s equation, Schrödinger–Newton equation, and by other names as well. Pekar [1] suggested it as an approximate model for H. Fröhlich’s condensed matter polaron [2], [3]; subsequently it was derived in a suitable limit $N \to \infty$ from $N$-body QM, see [4], [5], [6]. Choquard proposed it to characterize a self-trapped electron in a one-component quantum plasma; cf. [7], [8]. The name Schrödinger–Newton equation was coined by R. Penrose in his proposal that quantum-mechanical wave function collapse is caused by gravity [9]. It also occurs in the theory of hypothetical bosonic stars in the context of the dark matter mystery; it can be derived from QM of $N$ gravitating spin-zero bosons by taking a Hartree limit $N \to \infty$, see [10] and references therein. A survey of rigorous results for equation (1) and some of its generalizations is in [11].

Positive solutions to (1) minimize the functional

$$E(u) := \int_{\mathbb{R}^3} |\nabla u|^2(s)d^3s + \int_{\mathbb{R}^3} |u|^2(s)d^3s - \frac{1}{8\pi} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{|u^2(s)|u^2(s')}{|s-s'|}d^3sd^3s'$$

(2)

over the set of $u \in H^1(\mathbb{R}^3)$ under the Nehari condition that $u \neq 0$ satisfies $4\pi \int_{\mathbb{R}^3} (|\nabla u|^2(s) + |u|^2(s))d^3s = \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} |s-s'|^{-1}|u^2(s)|u^2(s')d^3s'd^3s'$ (obtained by multiplying (1) with $u$ and integrating over $\mathbb{R}^3$); this is equivalent to the usual minimization of r.h.s.(2) without $\int |u^2(s)d^3s$, yet under a normalization condition on this integral. It is known [7], [11] that any positive minimizer is radially symmetric about and decreasing away from an arbitrary point $s_0 \in \mathbb{R}^3$, and that for each $s_0$ there is a unique such solution. Moreover, since (1) and (2) are invariant under translations $s \mapsto s + a$, without loss of generality we assume that $s_0 = 0$, and (abusing notation) write $u(r)$ for $u(s)$ to denote this radially symmetric positive solution. We note that $u'(0) = 0$.

Interestingly, the somewhat delicate question of the asymptotic decay of positive minimizers has not yet been sorted out completely, as far as we can tell. D. Kumar and V. Soni in [12] claimed that there exists a positive constant $A$ such that (in our units) $u(r) = Ae^{-r} + \text{l.o.t.}$, where “l.o.t.” means “lower-order terms.” Based on their asymptotic analysis they concluded that (in units in which $\|u\|_2 = 1$) the energy coincides with that of the hydrogen atom, but a nonlocal quantity like an eigenvalue cannot be determined by a truncated asymptotic expansion, and indeed their energy claim was subsequently disproved in [13]. K. P. Tod and I. Moroz in [14] in turn claimed, though without proof, that if $u(r)$ is a positive radial solution to (1), then $u(r) = Ae^{-r}/r^{1-\|u\|_2^2/8\pi} + \text{l.o.t.}$; cf. (2.17a/b) in [14]. This claim was announced in [15] and repeated in [16]. What is proved in [14] is that for every positive $C < 1$ there are $A > 0$ and $b > 0$ such that $u(r) < Ae^{-Cr}/r^{1-\|u\|_2^2/8\pi}$ for all $r > b$, see Thm.3.1 in [14] (incidentally, a factor $e^{-b} \exp$ is obviously missing at r.h.s.(3.9) of [14]), but such an upper bound alone cannot establish the asymptotic behavior claimed in [14]. The question of the asymptotic behavior of $u(r)$ was taken up again by V. Moroz and J. van Schaftingen [17], who proved that the unique radially symmetric positive solution $u(r)$ to (1) obeys $\lim_{r \to \infty} r^{1-\|u\|_2^2/8\pi}e^{u(r)} \in (0, \infty)$; thus one has the asymptotic law $u(r) = Ae^{-r}/r^{1-\|u\|_2^2/8\pi} + \text{l.o.t.}$ for some $A > 0$; see their Thm.4, case $p = 2$ with $N = 3$ and $\alpha = 2$, and see also section 3.3.4 in [11]. However, the value of $\|u\|_2^2$ was left open in [17]. While the results of [17] rule out the asymptotic behavior claimed in [14], [15], and [16], it does leave open the possibility that the ground state solution of (1) perhaps decays as claimed in [12], i.e. purely exponentially like the hydrogen ground state (this would be the case if $\|u\|_2^2 = 8\pi$); but the exponential function could also have a decaying monomial factor (i.e. $\|u\|_2^2 < 8\pi$) or an increasing one (i.e. $\|u\|_2^2 > 8\pi$); in the latter case: is it concave (i.e. $\|u\|_2^2 < 16\pi$), linear ($\|u\|_2^2 = 16\pi$), or convex ($\|u\|_2^2 > 16\pi$)?

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With the help of rigorous energy bounds similar to those in [7] or [13], we prove

**Proposition 1.1** The $L^2$ norm of the positive $H^1$ solution $u(r)$ of (1) obeys the bounds

$$2^{1/3}3\pi^2 \leq \|u\|_2^2 \leq 8\pi^{3/2}. \quad (3)$$

This is strong enough to rigorously rule out the asymptotic form of $u(r)$ proposed in [12] (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 $e^{-r}$ increases in a strictly concave manner.

Although numerical studies of the Schrödinger–Newton equation have been carried out [15], [16], [18], 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 [18] by rescaling, revealing that the monomial prefactor of $e^{-r}$ is $\propto r^\beta$ with $\beta \approx 0.754$, i.e. increasing and strictly concave. We have carried out our own numerical study for (1) and directly computed that $\|u\|_2^2 \approx 14.03\pi$, compatible with the result extracted from [18] by rescaling.

Our upper bound in (3) is a factor $\approx 1.011$ too large compared to the numerically computed value.

**II. Rigorous Bounds on $\|u\|_2^2$**

In the following we prove Proposition 1.1.

**Proof:** For the purpose of our proof, and also for later convenience, we rescale (1) into

$$-\Delta \psi(s) - 2\int_{\mathbb{R}^3} \frac{1}{s-s'}|\psi|^2(s')d^3s' \psi(s) = E\psi(s), \quad (4)$$

in which form the Schrödinger–Newton equation appears in [7] and [18]; here, $\|\psi\|_2^2 = 1$. Equation (4) is the Euler–Lagrange equation for the minimization of the functional

$$\mathcal{F}(\psi) := \int_{\mathbb{R}^3} |\nabla \psi|^2(s)d^3s - \int_{\mathbb{R}^3} \frac{|\psi|^2(s)|\psi(s)|^2}{|s-s'|}d^3s d^3s'. \quad (5)$$

over the Sobolev space $H^1(\mathbb{R}^3)$ under the constraint $\int_{\mathbb{R}^3} |\psi|^2(s)d^3s = 1$; the eigenvalue $E$ is the Lagrange multiplier for this constraint; see [7].

Let $\psi_1(r)$ be the minimizer, and 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 $\frac{d}{d\lambda}\mathcal{F}(\psi_\lambda)|_{\lambda=1} = 0$ we obtain the virial identity

$$2\int_{\mathbb{R}^3} |\nabla \psi_1|^2(s)d^3s = \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{|\psi_1|^2(s)|\psi_1|^2(s')}{|s-s'|}d^3sd^3s'. \quad (6)$$

On the other hand, setting $\psi = \psi_1$ in (4), then multiplying (4) by $\psi_1$ and integrating over $\mathbb{R}^3$, one obtains

$$E_0 = \int_{\mathbb{R}^3} |\nabla \psi_1|^2(s)d^3s - 2\int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{|\psi_1|^2(s)|\psi_1|^2(s')}{|s-s'|}d^3sd^3s'. \quad (7)$$

for the ground state energy $E_0$. Now using (6) in (7) and also in (5), by comparison we obtain

$$E_0 = 3\mathcal{F}(\psi_1). \quad (8)$$

Thus, any upper or lower bounds on $\mathcal{F}(\psi_1)$ over $H^1$ under the normalization constraint $\|\psi_1\|_2 = 1$ translate into corresponding upper and lower bounds on the ground state energy $E_0$.

Next, by Sobolev’s inequality (cf. [13], p.174),

$$\int_{\mathbb{R}^3} \left(\frac{|\psi|^2(s)|\psi|^2(s')}{|s-s'|}\right)d^3s d^3s' \leq \frac{4}{3}\left(\int_{\mathbb{R}^3} |\psi|^2(s)d^3s\right)^{\frac{1}{3}} \left(\int_{\mathbb{R}^3} |\psi|^2(s')d^3s'\right)^{\frac{2}{3}}. \quad (10)$$

and Hölder’s inequality gives (cf. [13], p.175)

$$\int_{\mathbb{R}^3} |\psi|^2(s)d^3s \leq \left(\int_{\mathbb{R}^3} |\psi|^2(s)d^3s\right)^{\frac{3}{4}} \left(\int_{\mathbb{R}^3} |\psi|^6(s)d^3s\right)^{\frac{1}{4}}. \quad (11)$$

which simplifies because $\int_{\mathbb{R}^3} |\psi|^2(s)d^3s = 1$. Now setting $\int_{\mathbb{R}^3} |\psi|^6(s)d^3s =: x^6$, our chain of inequalities yields

$$\mathcal{F}(\psi_1) \geq 3\left[\frac{\pi}{2}\right]^\frac{3}{2} x^2 - 4\left[\frac{8}{3}\right]^\frac{1}{2} x; \quad (12)$$

and since we do not know $x$, to be on the safe side we minimize r.h.s.(12) w.r.t. $x > 0$ and obtain

$$\mathcal{F}(\psi_1) \geq -\frac{32}{27} \frac{2^{1/3}}{\pi^2} \approx -0.1513. \quad (13)$$

This yields

$$E_0 \geq -\frac{32}{27} \frac{2^{1/3}}{\pi^2} \approx -0.4539. \quad (14)$$

By rescaling the ground state energy to $E = -1$ we find $\|u\|_2^2 = 8\pi/\sqrt{|E_0|}$, and so, since $E_0 < 0$, by (14) we have

$$\|u\|_2^2 \geq 2^{1/3}3\pi^2 \approx 37.305. \quad (15)$$

This proves the lower bound in Proposition 1.1.

To obtain the upper bound in Proposition 1.1 we insert the Gaussian trial wave function $\psi_G(r) := \exp(-r^2/2R^2)/(\pi^{3/4}R^{3/2})$ into $\mathcal{F}(\psi)$ and minimize w.r.t. $R$, obtaining an upper bound on $\mathcal{F}(\psi_1)$. Rescaling to units in which the ground state energy $E = -1$ yields r.h.s.(3).

□

We end this section by remarking that our lower and upper bounds (3) are slightly stronger than those one can obtain from the energy bounds in [13] by scaling.
III. NUMERICAL ILLUSTRATION OF THE SCHRÖDINGER–NEWTON GROUND STATE

We have numerically computed an approximation to the Schrödinger–Newton ground state by dividing (1) by \( u(r) \), then applying \(-\Delta\), which by the radial symmetry yields a fourth-order ordinary differential equation for \( u(r) \), for which initial data \( u(0), u'(0), u''(0), \) and \( u'''(0) \) need to be supplied. From (1) one inherits \( u'(0) = 0 \), and well-posedness of the initial value problem for the fourth-order ODE requires \( u'''(0) = 0 \) also. This leaves \( u(0) > 0 \) and \( u''(0) \) to be determined such that \( u(r) > 0 \) for all \( r \geq 0 \), with \( \ln u(r) \sim -r \) as \( r \to \infty \), and \( u \in L^2(\mathbb{R}, r^2 dr) \). This single fourth-order ODE formulation is equivalent to the system of two second-order ODEs discussed in [14], [15], [16], and [18]. Fig. 1 shows the ground state \( u(r) \) and Fig. 2 its mass function \( M(r) := 4\pi \int_0^r |u(s)|^2 s^2 ds \). Note that \( \|u\|_2^2 = \lim_{r \to \infty} M(r) \).

![Ground state](image1.png)

**FIG. 1.** Shown is a numerical approximation to the ground state solution \( u(r) \) of (1).

![Mass of ground state in a ball of radius r](image2.png)

**FIG. 2.** Shown is \( M(r) := 4\pi \int_0^r |u(s)|^2 s^2 ds \) for the ground state solution \( u(r) \) of (1), together with the horizontal asymptote at \( 14.03\pi \approx \|u\|_2^2 = \lim_{r \to \infty} M(r) \).

Fig. 3, where we display the natural logarithm of \( u(r) \) together with a straight line of slope \(-1\), appears to suggest a purely exponential decay of the ground state \( u(r) \), but appearances are misleading, as visualized in Fig. 4.

![Logarithm of ground state](image3.png)

**FIG. 3.** Shown is the natural logarithm of the ground state solution \( u(r) \) of (1), together with a straight line of slope \(-1\).

![Logarithm of ground state plus Identity](image4.png)

**FIG. 4.** Shown is \( r + \ln u(r) \) versus \( r \) for the ground state solution \( u(r) \) of (1).

Fig. 4 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 \( u(r) \sim A \exp(-r) \). Instead, this map seems to behave \( \propto \ln r \) for large \( r \), which is confirmed in Fig. 5.

![Negative logarithm of ground state normalized by its asymptotic limit](image5.png)

**FIG. 5.** Shown is the negative natural logarithm of the ratio of the ground state solution \( u(r) \) of (1) over its asymptotic limit \( u_\infty(r) = Ar^\beta \exp(-r) \) with \( \beta \approx 0.754 \) and \( A \approx 3.37 \).
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 \(\ln u(r) \sim -r \) were terminated after a precision of three significant digits had been achieved, though.

As a test for our results we rescaled the ground state energy \(E = E_0\) for (4), computed numerically in [18] to be \(E_0 = -0.325(74)\), into our units in which the ground state energy \(E = -1\). This yields \(|u|^2 = 8\pi/\sqrt{|E_0|} \approx 44.09\), in good agreement with our result \(14.03\pi \approx 44.08\).

### IV. EXTERNAL \(-K/r\) POTENTIALS

In its bosonic star interpretation, the Schrödinger–Newton equation (1) captures the quantum-mechanical spin-zero bosons, in the Hartree limit \(N \to \infty\); cf. [10], and see [19] for a version with special-relativistic kinetic energy. Since these hypothetical building blocks of the mysterious dark matter will interact gravitationally with other matter, it is of interest to also consider the Schrödinger–Newton equation for bosons which are exposed to an external gravitational potential, which for simplicity we will assume to be radially symmetric and asymptotically \(\sim -K/r\) for some \(K > 0\). Incidentally, equipped with such an additional external \(-K/r\) potential the so-called generalized Schrödinger–Newton equation also can have bound states if the sign of the self-consistent interaction term (the cubic nonlinearity term at r.h.s.(1)) is changed from “+” to “−”. Therefore, in this and the next section we consider the equation

\[
-\Delta u(s) + u(s) = \frac{1}{4\pi} \int_{\mathbb{R}^3} \left[|u|^2 + |u|^2\right](s) \, d^3s + \frac{1}{8\pi} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{|u|^2(s)|u|^2(s')}{|s-s'|} \, d^3s \, d^3s' + \frac{3}{4\pi} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{|u|^2(s)|\mu(s')}{|s-s'|} \, d^3s \, d^3s' \tag{16}
\]

with \(\gamma > 0\) if the “+” sign is chosen, and in this section \(\gamma > 1\) if the “−” sign is; in the next section we also allow \(\gamma \geq 0.825\). Here, \(\mu(s) \geq 0\) is a given probability measure, in the following assumed to be radially symmetric. Eq.(16) with the “−” sign and \(\gamma > 1\) captures the ground state of a positive ion with hypothetical bosonic “electrons” in the Hartree limit \(N \to \infty\); cf. also [22], [23], [24], [25], [26], [27], and references therein. In that case \(\mu(s)\) represents the (normalized) charge distribution of the nucleus, which usually is modelled by a Dirac \(\delta\) measure but may also be considered to be bounded and radially symmetric decreasing. In the gravitational interpretation (i.e. “+” sign in (16)), \(\mu(s)\) is the normalized mass distribution of the other matter.

Eq.(16), with either sign, is the formal Euler–Lagrange equation for the minimization of the functional

\[
\mathcal{J}(u) := \int_{\mathbb{R}^3} \left([\nabla u]^2 + |u|^2\right)(s) \, d^3s + \frac{1}{8\pi} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{|u|^2(s)|u|^2(s')}{|s-s'|} \, d^3s \, d^3s' + \frac{3}{4\pi} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{|u|^2(s)|\mu(s')}{|s-s'|} \, d^3s \, d^3s' \tag{17}
\]

over the set of \(u \in H^1(\mathbb{R}^3)\) under the Nehari condition that \(u \neq 0\) satisfies \(4\pi \int_{\mathbb{R}^3} \left([\nabla u]^2(s) + |u|^2(s)\right) \, d^3s = \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} |s-s'|^{-1}|u|^2(s) \, [3||u|^2(s)|^2 + |u|^2(s')\right] \, d^3s \, d^3s'; \) no normalization condition on \(\int |u|^2(s) \, d^3s\) is imposed. Under our assumptions that \(\gamma > 0\) if the upper sign is chosen, and \(\gamma > 1\) if the lower one is, we may expect that a unique positive minimizer of \(\mathcal{J}(u)\) exists and satisfies (16), and in the following we assume this; cf. [28].

The asymptotic behavior of such a positive solution of (16) for rapidly decreasing \(\mu(r)\) (bounded by a Schwartz function) can be obtained by adapting the strategy of V. Moroz and J. van Schaftingen [17] to (16). We find

\[
\lim_{r \to \infty} r^{1-\gamma} \frac{1}{|u|^2 + 8\pi e^{-r} u(r)} \in (0, \infty); \tag{18}
\]

thus, \(u(r) = Ae^{-r}/r^{1-\gamma}\) for \(\gamma > 1\). Interestingly, (18) thus suggests that the asymptotic form of \(u(r)\) proposed by K. P. Tod and I. Moroz in [14] for (1) is instead true for the Hartree ground state of a neutral bosonic atom in the \(N \to \infty\) limit, when \(\gamma = 1\). In all the cases discussed in section IV the asymptotic form \(u(r) \sim Ae^{-r}/r^{\gamma/2}\) holds with \(\gamma < 1\).

Given that the question of the asymptotic decay of the Schrödinger–Newton ground state has received several conflicting answers until rigorous results showed the way, it is desirable to rigorously vindicate also the findings and the surmise reported in sections IV and V.

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statements in the published version (Phys. Lett. A 395, art. 127209 (2021)) have been omitted.

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