

Schrödinger-Newton solitons with axial symmetry

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We solve the Schrödinger-Newton problem of Newtonian gravity coupled to a nonrelativistic scalar particle for solutions with axial symmetry. The gravitational potential is driven by a mass density assumed to be proportional to the probability density of the scalar. Unlike related calculations for condensates of ultralight dark matter or boson stars, no assumption of spherical symmetry is made for the effective gravitational potential. Instead, the potential has only axial symmetry, consistent with the axial symmetry of the particle's probability density for eigenstates of L_z . With total angular momentum no longer a good quantum number, there are, in general, contributions from a range of partial waves. This permits us to study the partial-wave content of self-consistent solutions of the Schrödinger-Newton system.

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I. INTRODUCTION

We consider the states of a quantum particle bound in a gravitational well of its own making. The mass of the particle times its probability distribution provides the source for the Poisson equation that determines the Newtonian gravitational potential. The Schrödinger equation is then solved for this potential to find the particle's wave function. The self-consistent solution for a chosen energy level in the Schrödinger spectrum is then a soliton, a solitary wave. Previously, we [1] and others [2–8] considered solitons with spherical symmetry that are eigenstates of L^2 and L_z ; here we extend this to axial symmetry and eigenstates of L_z alone, with a more general treatment of this case than previously considered [9–19].

There are many applications for such solitons in astrophysics and cosmology. Ultralight dark matter [7,8,20–22] may form a Bose-Einstein condensate for which a Hartree-type analysis yields a single-particle wave function bound in an effective gravitational potential generated by all the other dark-matter particles. For nonrelativistic systems, this is mathematically equivalent to the Schrödinger-Newton system of equations as if each particle was bound by its own gravitational potential. The only quantitative difference is that, in the case of the condensate, the effective

potential is multiplied by the square of the number of particles.

The same mathematics arises in the case of boson stars [2,9–12,14,16,18,23,24]. Again, individual particles experience an effective potential derived from the mass distributions of all the others. This is extended to l -boson stars [15,17,19], where states with nonzero angular momentum l are filled in such a way that each angular momentum projection is equally likely, which guarantees a spherically symmetric source for the gravitational field. The gravitational potential is then spherically symmetric.¹ Axially symmetric solutions of the quantum eigenvalue problem are then obtained for this spherically symmetric potential.

On a more fundamental level, the Schrödinger-Newton problem also arose in the context of wave function collapse [25–27]. If the state of a system involves a superposition of two (or more) probability amplitudes with spatial separation, the gravitational interaction between the associated mass distributions should result in decay of the superposition over a time scale inversely related to the gravitational self-energy [28]. Such a superposition might decay into a Schrödinger-Newton soliton, and various calculations of these solitons have been done [3–6,13], primarily with an assumption of spherical symmetry.

The nonrelativistic problem is also obtained beginning with a semiclassical treatment of gravity [27], where the gravitational field is the solution to the equations of general relativity but the source is a stress-energy tensor computed

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¹In [16], spherical symmetry of the effective potential is implicit.

from quantum mechanical amplitudes. For a scalar particle, one can solve for the amplitude from the Klein-Gordon equation in curved spacetime [29] to obtain a self-consistent Einstein-Klein-Gordon soliton [1]. The nonrelativistic reduction of semiclassical gravity yields again the Schrödinger-Newton problem [30,31].

In this paper, we consider the Schrödinger-Newton problem in the more general situation of an axially symmetric gravitational potential. The wave functions are no longer necessarily eigenfunctions of L^2 but only of L_z . However, their simple $e^{im\phi}$ dependence on the azimuthal angle results in a probability density that is independent of the azimuthal angle.² The source for the gravitational potential is then axially symmetric, making the symmetry of the solutions self-consistent. Spherically symmetric solutions of this system are, of course, special cases, which we do reproduce.

With the azimuthal dependence trivial, the problem becomes two dimensional. We approach it in two ways. The first is as a set of two-dimensional partial differential equations, the Schrödinger equation and the Poisson equation.³ The second uses partial-wave expansions of the wave function and potential. For the former approach, we find serious problems with convergence of the iteration for self-consistency except for the ground state, unless the initial guess is very close to the final result. Convergence in the case of the partial-wave expansions is quite rapid, requiring on the order of 20 iterations to achieve accuracy consistent with the underlying numerical methods for the differential equations. Results from this method are confirmed by using the first method starting from interpolations of the solution from the second method, which is then usually sufficient to obtain convergence.

Our approach differs from earlier work with partial waves [10]. There the sum was restricted to a single partial wave that was assumed to be dominant. We instead sum over all partial waves that make any significant contribution and tabulate the range of contributions. In doing so, we found a case where two partial waves were equally important.

The poor convergence of the first method appears to be due to the fact that a self-consistent solution can exist anywhere in space; there is no predetermined location for the “center” of the soliton. Within the restriction to cylindrical coordinates, and with the assumption of cylindrical symmetry with respect to these coordinates, the soliton is still able to appear anywhere along the symmetry axis. In any excited state, there are secondary peaks in the wave function that can confuse the numerical algorithm into seeing them as a central source, and the iteration seeks

to find a solution at each new location along the axis of symmetry. The partial-wave expansion defeats this because any secondary peaks in radial wave functions correspond to spherical shells rather than new centers.

A mathematical description of the Schrödinger-Newton problem is given in Sec. II, where we also describe our methods of solution. Results are presented in Sec. III and summarized in Sec. IV. Details of the numerical methods are given in the Appendix.

II. SCHRÖDINGER-NEWTON PROBLEM

Given the Hamiltonian $H = -\frac{1}{2m}\nabla^2 + V$, with $V = m\Phi$ the potential energy in a gravitational potential Φ , the coupled system is

$$H\psi = E\psi, \quad \nabla^2\Phi = 4\pi Gm|\psi|^2. \quad (2.1)$$

Here $m|\psi|^2$ is taken to be the mass density. We assume axial symmetry so that Φ is independent of the azimuthal angle ϕ and H commutes with L_z . The wave function is then an eigenstate of L_z and takes the form $\frac{1}{\sqrt{2\pi}}R_{m_l}(\rho, z)e^{im_l\phi}$, with z the symmetry axis and ρ the radial distance from it. The mass density is just $\frac{m}{2\pi}|R_{m_l}(\rho, z)|^2$ and also independent of azimuthal angle.

We also assume that the gravitational potential $\Phi(\rho, z)$ is even with respect to reflection in z . The Hamiltonian is then invariant in z parity, and the eigenfunctions R_{m_l} can be chosen even or odd. This makes the source of the gravitational potential even and self-consistent with the chosen symmetry of the potential.

Solutions with spherical symmetry are recovered as a subset of those solutions with $m_l = 0$. We use this as a partial check on the calculations. A second check is to compare results from solving the system in two ways, one using cylindrical coordinates ρ and z , as already introduced, and the other using spherical coordinates r and θ , with $z = r \cos \theta$ and $\rho = r \sin \theta$ as usual.

A. Cylindrical coordinates

In cylindrical coordinates, the Schrödinger equation reduces to

$$-\frac{1}{2m}\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial R_{m_l}}{\partial\rho}\right) - \frac{m_l^2}{\rho^2}R_{m_l} + \frac{\partial^2 R_{m_l}}{\partial z^2}\right] + V_{m_l}(\rho, z)R_{m_l} = E_{m_l}R_{m_l}, \quad (2.2)$$

and, when written in terms of the potential energy $V = m\Phi$, the Poisson equation for Newtonian gravity becomes

$$\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial V_{m_l}}{\partial\rho}\right) + \frac{\partial^2 V_{m_l}}{\partial z^2} = 2Gm^2|R_{m_l}|^2. \quad (2.3)$$

The wave function is normalized as

²Harrison [13] assumed wave functions independent of the azimuthal angle, but this is unnecessarily restrictive.

³Schupp and Van der Bij [9] approach the problem in this way; we agree with their only nonspherical result.

$$1 = \int \rho d\rho dz d\phi |\psi|^2 = \int \rho d\rho dz |R_{m_l}|^2, \quad (2.4)$$

so that the total mass is m with a density of $m|\psi|^2$.

To have a dimensionless representation, as discussed elsewhere [1,29], we rescale lengths by the gravitational Bohr radius $a = 1/\text{Gm}^3$, energies by $\text{G}^2 \text{m}^5$, with $\epsilon_{m_l} \equiv E_{m_l}/\text{G}^2 \text{m}^5$, and the wave function by $a^{-3/2} = (\text{Gm}^3)^{3/2}$ to obtain in the same notation

$$-\frac{1}{2} \left[\frac{1}{\rho} \frac{\partial}{\partial \rho} \left(\rho \frac{\partial R_{m_l}}{\partial \rho} \right) - \frac{m_l^2}{\rho^2} R_{m_l} + \frac{\partial^2 R_{m_l}}{\partial z^2} \right] + V_{m_l}(\rho, z) R_{m_l} = \epsilon_{m_l} R_{m_l} \quad (2.5)$$

and

$$\frac{1}{\rho} \frac{\partial}{\partial \rho} \left(\rho \frac{\partial V_{m_l}}{\partial \rho} \right) + \frac{\partial^2 V_{m_l}}{\partial z^2} = 2|R_{m_l}|^2. \quad (2.6)$$

Given all the rescalings, the normalization expression is invariant,

$$1 = \int \rho d\rho dz |R_{m_l}|^2. \quad (2.7)$$

It is also convenient to introduce the reduced wave function $u_{m_l} \equiv \sqrt{\rho} R_{m_l}$ for which the two-dimensional Schrödinger equation becomes

$$-\frac{1}{2} \left[\frac{\partial^2 u_{m_l}}{\partial \rho^2} - \frac{m_l^2 - 1/4}{\rho^2} u_{m_l} + \frac{\partial^2 u_{m_l}}{\partial z^2} \right] + V_{m_l}(\rho, z) u_{m_l} = \epsilon_{m_l} u_{m_l}. \quad (2.8)$$

However, for $m_l = 0$ the boundary condition $u_{m_l}(\rho = 0, z) = 0$ is difficult to maintain numerically; cancellations between the $1/4\rho^2$ term and finite-difference expressions for the partial derivatives with respect to ρ are imprecise near $\rho = 0$. In this case, the original equation for R_0 is the better route despite the more complicated ρ derivatives.

To solve each of the equations in the system, we apply finite-difference approximations for all derivatives on a finite grid and study the dependence on grid spacing and grid size. The finite-difference representation of the Schrödinger equation is solved as a matrix eigenvalue problem and that of the Poisson equation is solved with the usual successive-overrelaxation method. The coupled system is then solved iteratively, starting from an initial guess for the wave function, until both R_{m_l} and V_{m_l} converge to consistent solutions. This requires a choice of energy level from the multiple solutions of the Schrödinger eigenvalue problem; each generates its own unique gravitational potential because each energy level has a different wave function and therefore a different probability distribution.

One aspect that is important to note is that, although the grid is chosen large enough for the wave function to be effectively zero at the boundary, the potential V does not

fall nearly fast enough to be well approximated by zero there. Instead, we represent V by a truncated multipole expansion computed from the mass distribution under the assumption that all the mass is contained within the grid. Once the moments of the mass distribution are computed, the value of V along the boundary can be estimated. In our rescaled units, the multipole expansion is

$$V_{m_l}(\rho, z) = -\sum_l \frac{Q_{lm_l}}{(\sqrt{\rho^2 + z^2})^{l+1}} P_l\left(z/\sqrt{\rho^2 + z^2}\right), \quad (2.9)$$

with moments

$$Q_{lm_l} = \int \left(\sqrt{\rho^2 + z^2}\right)^l \rho d\rho dz P_l\left(z/\sqrt{\rho^2 + z^2}\right) |R_{m_l}|^2 \quad (2.10)$$

and P_l the Legendre polynomial of order l . The leading term in V_{m_l} is $-1/r$, the 1 being the normalization of R_{m_l} . For odd l , the moments are zero because $|R_{m_l}|^2$ is even in z . The other moments are computed numerically with trapezoidal approximations to the integrals.

As discussed in the Introduction, the convergence of the system iteration is problematic. Except for the spherically symmetric ground state, the iteration typically requires a very good estimate for the initial guess. We therefore use the formulation in cylindrical coordinates as a check on our method for spherical coordinates. Further details of the numerical approach are given in the Appendix.

B. Spherical coordinates

In terms of spherical coordinates, the natural approach is one of partial waves.⁴ By expanding both the wave function and the potential in terms of spherical harmonics, one can obtain coupled sets of ordinary differential equations for the expansion coefficients, which are functions of the radial distance r . To have a finite set of equations, the expansion is truncated at a maximum value $l_{\max}$ for the angular momentum quantum number l ; of course, the dependence on $l_{\max}$ must be checked. The coefficient functions for different l are coupled, in general, because the potential is only axially symmetric, not spherically symmetric.

The partial-wave expansions are

$$\begin{aligned} \psi_{m_l}(r, \theta, \phi) &= \sum_{l=|m_l|}^{l_{\max}} \frac{u_{lm_l}(r)}{r} Y_{lm_l}(\theta, \phi), \\ V_{m_l}(r, \theta) &= \sum_{l=0}^{l_{\max}} \frac{v_{lm_l}(r)}{r} Y_{l0}(\theta). \end{aligned} \quad (2.11)$$

⁴As mentioned in the Introduction, this approach was used in [10], but the sum over partial waves was restricted to a single partial wave, assumed to be dominant.

For ψ , only l values with $l - |m_l|$ even (odd) contribute to states even (odd) in $z = r \cos \theta$, as determined by the associated Legendre functions in the Y_{lm_l} . For V , only Y_{l0} with l even contribute because V is independent of ϕ and even in z .

With the definition of the overlap integrals

$$C_{l,l'l''}^{m_l} \equiv \int d\Omega Y_{lm_l}^* Y_{l'0} Y_{l''m_l}, \quad (2.12)$$

the coupled systems are

$$-\frac{1}{2} \frac{d^2 u_{lm_l}}{dr^2} + \frac{l(l+1)}{2r^2} u_{lm_l} + \frac{1}{r} \sum_{l',l''}^{l_{\max}} C_{l,l'l''}^{m_l} v_{l'm_l} u_{l''m_l} = \epsilon_{m_l} u_{lm_l} \quad (2.13)$$

and

$$\frac{d^2 v_{lm_l}}{dr^2} - \frac{l(l+1)}{r^2} v_{lm_l} = \frac{4\pi}{r} \sum_{l',l''} C_{l,l'l''}^{m_l*} u_{l'm_l} u_{l''m_l}. \quad (2.14)$$

Again, a grid is introduced, though only one dimensional in this case, out to a finite range of $r_{\max}$, and the equations are replaced by finite-difference approximations. The system

for the u_{lm_l} is solved as a matrix eigenvalue problem for the chosen level and z parity at a fixed value of m_l . The system for the v_{lm_l} is not coupled between different l and each (inhomogeneous) finite-difference equation is solved as a linear system. The overlap integrals are computed from Clebsch-Gordan coefficients with use of the Python procedure `sympy.physics.quantum.cg`; the connection is

$$C_{l,l'l''}^{m_l} = \sqrt{\frac{(2l'+1)(2l''+1)}{4\pi(2l+1)}} \times \langle l'l''00 | (l'l'')l0 \rangle \langle l'l''0m_l | (l'l'')lm_l \rangle. \quad (2.15)$$

The boundary conditions for these systems are

$$u_{lm_l}(0) = 0, \quad u_{lm_l}(r_{\max}) = 0 \quad (2.16)$$

and

$$v_{lm_l}(0) = 0, \quad v_{lm_l}(r_{\max}) = -\sqrt{\frac{4\pi}{2l+1}} \frac{Q_{lm_l}}{r_{\max}^l}, \quad (2.17)$$

with Q_{lm_l} defined in (2.10). As in the case of cylindrical coordinates, the boundary condition for v_{lm_l} at $r_{\max}$ comes from a comparison with the multipole expansion in the

TABLE I. Eigenenergies in units of $G^2 m^5$ for low-lying states at fixed m_l and z parity even or odd, computed on a grid from 0 to $r_{\max}$ with step size h in a partial-wave expansion truncated at $l_{\max}$. Typical values for the computational parameters are $80a$ – $160a$ for $r_{\max}$ and $l_{\max} = 10$, with h small enough to achieve four significant figures. Only those states that fall within the energy range of the $m_l = 0$, z even subset are tabulated.

$m_l = 0$		$m_l = 1$		$m_l = 2$	
Even	Odd	Even	Odd	Even	Odd
−0.1628	−0.06894	−0.05710	−0.02900	−0.03066	−0.01712
−0.03082	−0.0274	−0.01928	−0.01402	−0.01312	
−0.0252	−0.0169				
−0.01254					

TABLE II. Partial-wave content of low-lying states with contributions from even l values, for various m_l values and z parities. The eigenenergies ϵ_{m_l} are in units of $G^2 m^5$. The m_l value and z parity determine the contributing partial waves as those with $l - m_l$ even (odd) for z parity even (odd).

m_l	z parity	ϵ_{m_l}	l for partial wave					
			0	2	4	6	8	10
0	Even	−0.1628	1					
0	Even	−0.03082	1					
0	Even	−0.0252	0.7128	0.2576	0.02731	0.002217	6.13×10^{-5}	1.18×10^{-6}
0	Even	−0.01254	1					
1	Odd	−0.02900		0.9837	0.01605	0.0002743	1.95×10^{-5}	4.0×10^{-9}
1	Odd	−0.01402		0.4505	0.4559	0.08598	0.007410	0.000240
2	Even	−0.03066		0.9794	0.02021	0.0004160	7.82×10^{-6}	1.37×10^{-7}
2	Even	−0.01312		0.8752	0.1125	0.01128	0.0009063	6.51×10^{-5}

TABLE III. Same as for Table II but for states with contributions from odd l values.

m_l	z parity	ϵ_{m_l}	l for partial wave				
			1	3	5	7	9
0	Odd	-0.06894	0.9363	0.06193	0.001765	3.63×10^{-5}	6.34×10^{-7}
0	Odd	-0.0274	0.5940	0.3306	0.06479	0.009440	0.001250
0	Odd	-0.0169	0.6892	0.3000	0.01040	3.000×10^{-4}	1.23×10^{-4}
1	Even	-0.05710	0.9936	0.006389	2.47×10^{-5}	7.46×10^{-8}	2.0×10^{-10}
1	Even	-0.01928	0.8531	0.1376	0.008862	0.0004453	1.99×10^{-5}
2	Odd	-0.01712		0.9978	0.0007470	0.001440	8.4×10^{-6}

region outside the source. In spherical coordinates, this expansion is

$$V_{m_l}(r, \theta) = -\sum_l \frac{Q_{lm_l}}{r^{l+1}} P_l(\cos \theta), \quad (2.18)$$

and the moments are written as

$$Q_{lm_l} = \int r^{l+2} dr d(\cos \theta) d\phi P_l(\cos \theta) |\psi|^2. \quad (2.19)$$

Given the partial-wave expansion for ψ in (2.11), the moments reduce to

$$Q_{lm_l} = \sqrt{\frac{4\pi}{2l+1}} \sum_{l', l''=|m_l|}^{l_{\max}} C_{l', l''}^{m_l} \int r^l dr u_{l' m_l} u_{l'' m_l}. \quad (2.20)$$

The leading factors depending on 4π and $2l+1$ are due to the connection $Y_{l0} = \sqrt{\frac{2l+1}{4\pi}} P_l$.

Because each partial wave is orthogonal, the normalization condition for the radial wave functions is just a simple sum of integrals,

$$1 = \sum_{l=|m_l|}^{l_{\max}} \int dr |u_{lm_l}|^2. \quad (2.21)$$

This determines an overall normalization constant. The relative normalization for each l is determined by the solution of the eigenvalue problem.

The combination of the partial-wave equations for the radial wave functions and the potential energy functions is again solved iteratively, beginning with a simple Gaussian as the initial guess for the lowest partial wave. Convergence to four significant figures typically requires 20 iterations. Additional details are given in the Appendix.

III. RESULTS

We have used these methods to compute some low-lying eigenstates for m_l values 0, 1, and 2 and for both z parities.

The energies are listed in Table I. The relative probabilities of the partial waves are presented in Tables II and III. States with energies outside the range of the energies in the first column of Table I certainly exist but were not considered. The probability densities obtained in each case are plotted in Figs. 1–4. As expected, an increase in the energy or the

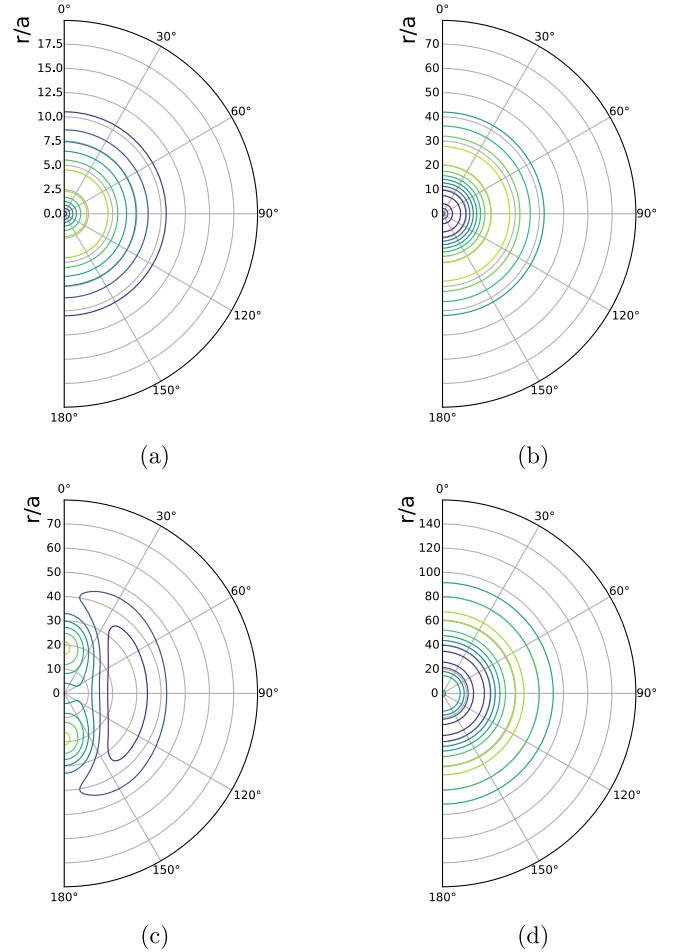


FIG. 1. Probability densities for the four lowest-lying states with $m_l = 0$ and even z parity. The associated eigenenergies in units of $G^2 m^5$ are (a) -0.1628 , (b) -0.03082 , (c) -0.0252 , and (d) -0.01254 . Only (c) is not spherically symmetric.

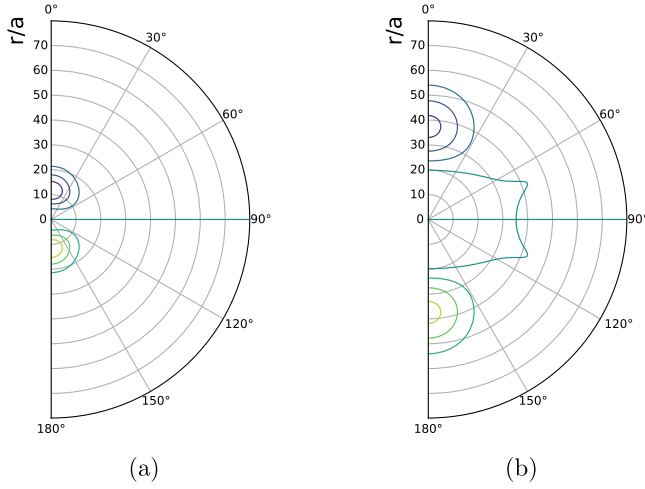


FIG. 2. Probability densities for the three lowest-lying states with $m_l = 0$ and odd z parity. The associated eigenenergies in units of $G^2 m^5$ are (a) -0.06894 , (b) -0.0274 , and (c) -0.0169 .

m_l value brings an increase in the complexity of the probability distributions.

The eigenenergies of the spherically symmetric states agree with those calculated previously [1]. These are the first, second, and fourth energies listed in the first column of Table I. A state with only axial symmetry has appeared in that column as the third entry; Table II shows its partial-wave content, with a 26% probability for $l = 2$.

One interesting aspect of the spectrum is that the first excited state is not spherically symmetric. It is instead odd in z with an energy of $-0.06894 G^2 m^5$ and $m_l = 0$. Only odd l partial waves contribute, beginning with $l = 1$, and with a 6.2% probability for $l = 3$. The probability density is plotted in Fig. 2(a). The energy of this state agrees with the result obtained by Schupp and Van der Bij [9].⁵

⁵One must take into account their different definition of a dimensionless energy $\hat{E} = -\epsilon/2$.

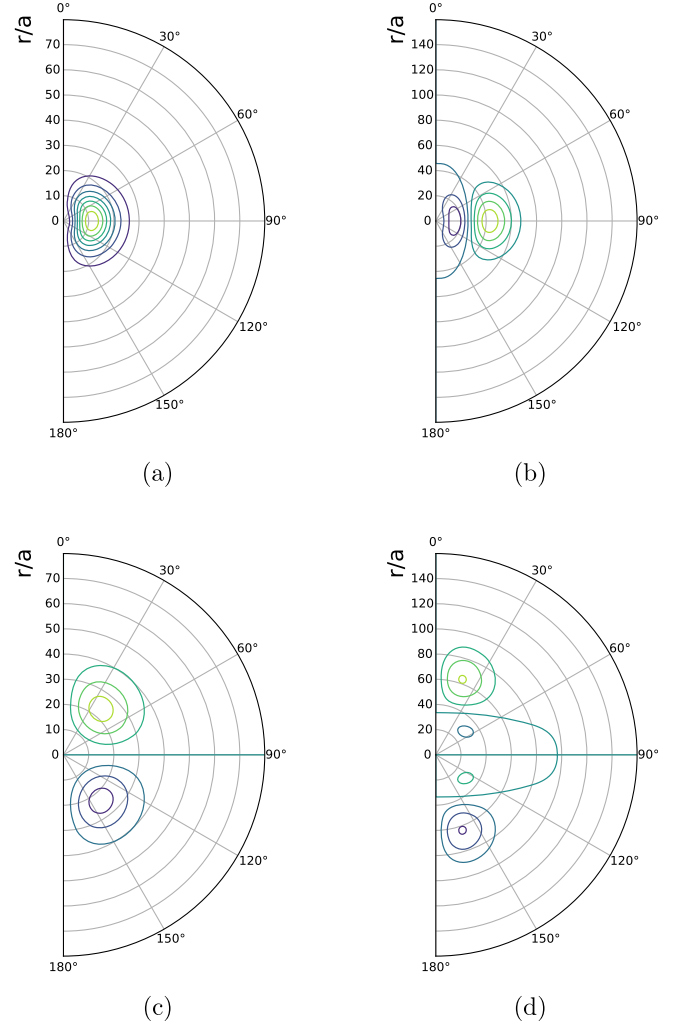


FIG. 3. Probability densities for the four lowest-lying states with $m_l = 1$. The associated z parities and eigenenergies in units of $G^2 m^5$ are (a) even, -0.05710 ; (b) even, -0.01928 ; (c) odd, -0.02900 ; and (d) odd, -0.01402 .

The state with perhaps the most interesting structure is the odd $m_l = 1$ state depicted in Fig. 3(d) with an energy of $-0.01402 G^2 m^5$. The probability density has four peaks and a partial-wave content of 45% for $l = 2$, 46% for $l = 4$, and 8.6% for $l = 6$. It is the only state, of those computed, where the second partial wave is as important as the first. It is also an example of why restriction to a single partial wave, as done in [10], will not always provide a good approximation.

Any state with a partial-wave content for $l \geq 2$ can transition to a lower state by emitting a gravitational wave, which has helicity ± 2 . Thus, many of the computed states are actually unstable to radiation [24]. This is in contrast to the instability of l -boson stars for l as low as 1 as discussed, for example, in [18]. An l -boson star is a multiparticle system with more transition pathways available than the single-particle system considered here.

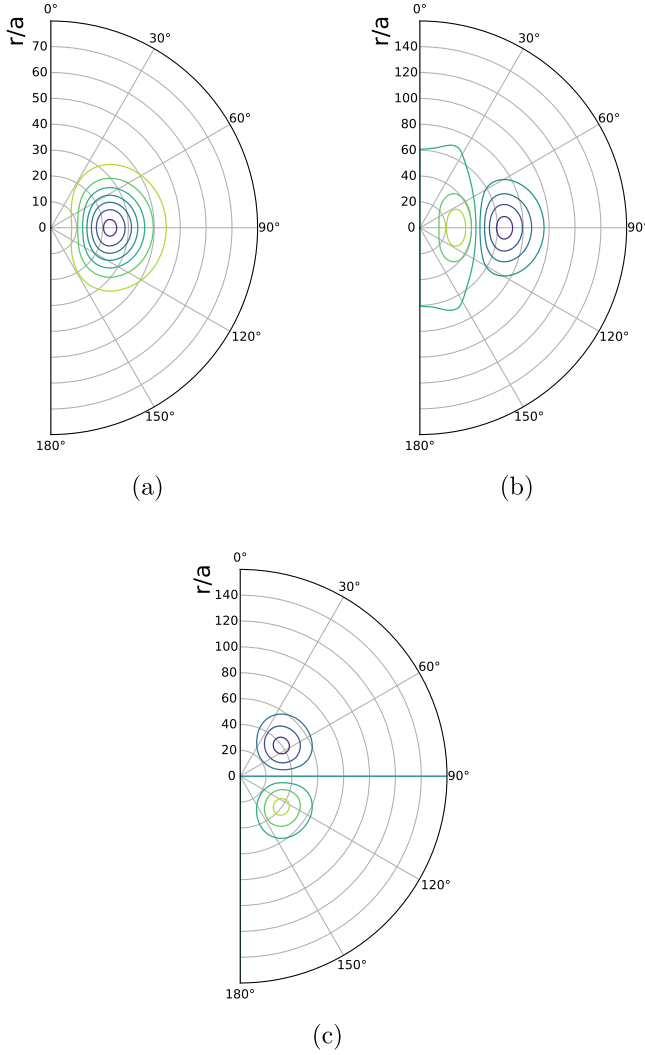


FIG. 4. Probability densities for the three lowest-lying states with $m_l = 2$. The associated z parities and eigenenergies in units of $G^2 m^5$ are (a) even, -0.03066 ; (b) even, -0.01312 ; and (c) odd, -0.01712 .

Unstable states could, in principle, be created by graviton absorption from a lower, stable state. Lifetimes for these states could be computed, but that is beyond the scope of the present work.

IV. SUMMARY

We have solved the Schrödinger-Newton problem for solitons with axial symmetry using partial-wave expansions that show the range of angular momentum content. The energies obtained are listed in Table I and include several spherically symmetric states previously computed. The partial-wave content of each state is listed in Table II or III, depending on whether the content is even or odd in l , respectively. Plots of the mass distributions are given in Figs. 1–4 and show significant structure for those lacking spherical symmetry. Some interesting aspects of the

spectrum and states are the presence of a nonspherical solution as the third state with azimuthal quantum number $m_l = 0$, the first excited state being one without spherical symmetry, and a state ($E = -0.01402 G^2 m^5$) with nearly equal contributions from $l = 2$ and $l = 4$ partial waves.

The methods employed provide a more complete picture of these solitons than previously obtained, in that the sum over partial waves includes any with significant contribution rather than approximating with a single partial wave [10]. The calculations also extend the study of axially symmetric solitons to cases where the effective potential is not spherically symmetric, as is typically arranged for the study of I -boson stars [15,17,19].

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DATA AVAILABILITY

The data that support the findings of this article are openly available [32].

APPENDIX: DETAILS OF NUMERICAL METHODS

For the method in cylindrical coordinates, the coupled system of Schrödinger and Poisson equations was solved self-consistently by iterating between the individual equations, starting from an initial guess for the wave function for which the potential was computed, and cycling between equations until the eigenvalue of the chosen state converged to within 10^{-5} . For the ground state, a simple Gaussian initial wave function was sufficient to achieve convergence. As discussed in the Introduction, convergence for excited states required an initial wave function that was close to the solution; this was obtained by the method in spherical coordinates and then linearly interpolated for the cylindrical grid. Also, in the first pass through the iterations, the successive overrelaxation (SOR) iterations to solve the Poisson equation were started with an interpolation of the potential obtained as the solution in the method for spherical coordinates; in subsequent iterations, the SOR method started from the potential obtained in the previous iteration. The SOR convergence requirement was that the maximum change in the potential across the grid be less than 10^{-8} , and the SOR parameter ω was set to a value of 1.2.

The matrix eigenvalue problem that represented the Schrödinger equation was solved with the Python sparse algebra routines `scipy.sparse.linalg.eigs` and `eigsh`. The latter was used only for $m_l = 0$ with odd z parity, for which the matrix representation was symmetric. Both are based on earlier ARPACK routines that use the implicitly restarted Arnoldi method. The Python codes that

carry out these and all other calculations are publicly available [32].

The number of grid points ranged no higher than 200 in each of the radial and z directions. Larger values made the matrix representation quite large and run times quite long, and, given that this method was used only to confirm the results in spherical coordinates rather than to reach complete convergence, such larger values were deemed unnecessary. All of the reported results come from calculations with spherical coordinates.

For the method in spherical coordinates, the iterations were structured in the same way as for cylindrical coordinates. The initial guess for the wave function was a Gaussian shape with the correct z parity in the lowest partial wave and no content in higher partial waves. Iterations continued until the eigenvalue of the chosen state again reached a tolerance of 10^{-5} . The linear equations for the potential were solved with the Python routine `numpy.linalg.solve`, and the eigenvalue problem for the partial waves was solved by `scipy.linalg.eigh`, which is based on the EVR method in LAPACK that begins with reduction to a tridiagonal form.

Up to 1600 grid points were used in the radial direction, and the truncated sum over partial waves was increased to 10.

The radial grid size ranged up to 160, in multiples of the Bohr radius, with the larger grid sizes needed for the excited states, of course. In each case, calculations were done for a succession of grid sizes at fixed grid spacing, and then repeated for decreased grid spacings, until four significant figures were achieved in the eigenvalue. Variation in the truncation of the partial-wave sum was also considered, to check for sensitivity to this numerical parameter. Finally, the results obtained were checked against results from the method based on cylindrical coordinates, to confirm values at an approximate level and to guard against spurious solutions.

The matrix representation for the coupled radial Schrödinger equations is a Rayleigh-Ritz variational approximation that truncates an infinite basis to a finite size. As such, the precision of the wave function values is less than that of the eigenvalues, particularly for higher partial waves with low probability. Tables II and III report probabilities for partial waves that are obtained by summing squares of individual wave function values and thereby averaging over errors in individual wave function values. The probabilities of higher partial waves are given with fewer significant figures; however, they provide clear indications of the relative (un)importance of higher partial waves for low-lying states.

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