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Rational Chebyshev series for the Thomas-Fermi function: endpoint singularities and spectral methods. (English) Zbl 1260.65065

Summary: We solve the Thomas-Fermi problem for neutral atoms, $u_{yy} - (1/\sqrt{y})u^{3/2} = 0$ on $y \in [0, \infty]$ with $u(0) = 1$ and $u(\infty) = 0$, using rational Chebyshev functions $T_Ln(y; L)$ to illustrate some themes in solving differential equations on a semi-infinite interval. $L$ is a user-choosable numerical parameter. The Thomas-Fermi equation is singular at the origin, giving a $T_L$ convergence rate of only fourth order, but this can be removed by the change of variables, $z = \sqrt{y}$ with $v(z) = \sqrt{u(y(z))}$. The function $v(z)$ decays as $z \to \infty$ with a term in $z^{-3}$, which is consistent with a geometric rate of convergence. However, the asymptotic series has additional terms with irrational fractional powers beginning with $z^{-4.544}$. In spite of the faster spatial decay, the irrational powers degrade the convergence rate to slightly larger than tenth order. This vividly illustrates the subtle connection between the spatial decay of $u(x)$ and the decay-with-degree of its rational Chebyshev series. The $TL$ coefficients $a_n(L)$ are hostages to a tug-of-war between a singularity on the negative real axis, which gives a geometric rate of convergence that slows with increasing $L$, and the slow inverse power decay for large $z$, which gives quasi-tenth order convergence with a proportionality constant that decreases inversely as a power of $L$. For $L = 2$, we can approximate $u_y(0) (= v_{zz}(0))$ to 1 part in a million with a truncation $N$ of only 20. $L = 64$ and $N = 600$ gives $u_y(0) = -1.5880710226113753127186845$, correct to 25 decimal places.

MSC:
65L10 Numerical solution of boundary value problems involving ordinary differential equations
34B15 Nonlinear boundary value problems for ordinary differential equations
65L60 Finite element, Rayleigh-Ritz, Galerkin and collocation methods for ordinary differential equations
65L20 Stability and convergence of numerical methods for ordinary differential equations

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Software:
DLMF

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