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VARIATIONAL SOLUTIONS OF THE THOMAS-FERMI EQUATION*

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Abstract. Variational solutions of the Thomas-Fermi equation are examined in the context of complementary extremum principles. A new one-parameter trial function is found to provide an accurate representation of the solution.

1. Introduction. The Thomas-Fermi screening function $\phi(x)$ for neutral atoms with spherical symmetry satisfies the nonlinear second-order differential equation (see [6])

$$d^2\phi/dx^2 = \phi^{3/2}/x^{1/2}, \qquad 0 \le x < \infty, \tag{1}$$

subject to the boundary conditions

$$\phi(0) = 1; \qquad \phi \to 0, \qquad x\phi' \to 0 \quad \text{as} \quad x \to \infty. \tag{2}$$

Near $x = 0$ the function $\phi(x)$ can be expanded as

$$\phi(x) = 1 + cx + \tfrac{4}{3}x^{3/2} + \tfrac{2}{5}cx^{5/2} + \tfrac{1}{3}x^3 + \cdots, \tag{3}$$

where c is the unspecified value of $\phi'(0)$, while for large x the solution behaves like

$$\phi(x) \sim 144/x^3 \quad \text{as} \quad x \to \infty. \tag{4}$$

An analytical solution of the problem in (1) and (2) is not known and so recourse must be taken in approximate solutions. Such solutions are either purely numerical [3, 5] or variational [4, 7]. Here we shall be concerned with solutions of the latter kind.

From the theory of complementary variational principles (see [2]) we find that the solution ϕ of (1) and (2) is the function which minimizes the integral

$$J(\Phi) = \int_0^\infty \left\{ \frac{1}{2}(\Phi')^2 + \frac{2}{5}\frac{\Phi^{5/2}}{x^{1/2}} \right\} dx, \tag{5}$$

and which maximizes the integral

$$G(\Psi) = -\int_0^\infty \left\{ \frac{1}{2}(\Psi')^2 + \frac{3}{5}\frac{(x^{1/2}\Psi'')^{5/3}}{x^{1/2}} \right\} dx - \Psi'(0). \tag{6}$$

The extreme values of J and G agree and we have the global upper and lower bounds

$$G(\Psi) \le G(\phi) = J(\phi) \le J(\Phi). \tag{7}$$

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Here the trial function Φ is subject to conditions (2) while the trial function Ψ is free of essential conditions. The extremum principles in (7) provide a basis for variational approximations to the exact function ϕ, the difference J-G being a measure of the accuracy of Φ and Ψ.

2. Variational solutions. The trial function

$$\Phi_1 = \{ae^{-\alpha x} + be^{-\beta x}\}^2, \qquad a + b = 1, \tag{8}$$

has been proposed by Csavinsky [4] who determined the three free parameters by a method equivalent to minimizing $J(\Phi_1)$, with the results

$$J = 0.6816 \tag{9}$$

at $a = 0.7111$, $\alpha = 0.175$, $\beta = 9.5\alpha$. For the same class of trial functions the optimum value of the complementary integral G is [1]

$$G = 0.6010. \tag{10}$$

An improvement on these results is provided by the one-parameter trial function

$$\Phi_2 = (1 + \gamma x^{1/2})e^{-\gamma x^{1/2}} \tag{11}$$

of Roberts [7], who found the minimum value of $J(\Phi_2)$ to be

$$J = 0.6810 \quad \text{at} \quad \gamma = 1.905. \tag{12}$$

The optimum value of G for the same class of trial functions is [1]

$$G = 0.6699 \quad \text{at} \quad \gamma = 1.750. \tag{13}$$

Neither function Φ_1 nor Φ_2 has the correct behavior for large x, while for small x, where the function is most significant, Φ_1 has an expansion involving only integral powers of x and cannot look like (3), and Φ_2 has the expansion

$$\Phi_2 = 1 - \tfrac{1}{2}\gamma^2 x + \tfrac{1}{3}\gamma^3 x^{3/2} - \tfrac{1}{8}\gamma^4 x^2 + \left(\frac{1}{4!} - \frac{1}{5!}\right)\gamma^5 x^{5/2} + O(x^3). \tag{14}$$

Comparison of (14) with (3) shows that these expressions agree on the absence of a term in $x^{1/2}$, but that Φ_2 contains a term in x^2 which is not present in (3). To incorporate this feature of the exact function ϕ near $x = 0$, and to retain expansion in powers of $x^{1/2}$, we shall therefore modify Φ_2 in (11) in the simplest possible way and introduce the one-parameter class of trial functions

$$\Phi_3 = (1 + \alpha x^{1/2} + \tfrac{1}{4}\alpha^2 x)e^{-\alpha^2}x)e^{-\alpha x^{1/2}}. \tag{15}$$

Near $x = 0$ such a trial function has the expansion

$$\Phi_3 = 1 - \tfrac{1}{4}\alpha^2 x + \tfrac{1}{12}\alpha^3 x^{3/2} - \frac{1}{5!}\alpha^5 x^{5/2} + \frac{1}{4!\,12}\alpha^6 x^3 + O(x^{7/2}), \tag{16}$$

the terms in $x^{1/2}$ and x^2 being absent as required.

With function Φ_3 the optimum values of J and G and the variational parameter α are

$$J = 0.6811 \quad \text{at} \quad \alpha = 2.472, \tag{17}$$

$$G = 0.6803 \quad \text{at} \quad \alpha = 2.528. \tag{18}$$

In terms of the agreement of these bounds the variational solution Φ_3 is the best of the three trial functions. Comparison with the numerical solution [3] shows a discrepancy of less than one percent in the region $0 \leq x \leq 1$ where the function drops from 1 to 0.4. For $x > 1$, Φ_3 falls off more rapidly than the numerical solution, but this behavior is to be expected through the built-in exponential decrease in the trial function.

References

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