A VARIATIONAL-ITERATIVE APPROXIMATE SOLUTION OF THE THOMAS-FERMI EQUATION*

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Abstract. Variational-iterative solutions of the Thomas-Fermi equation are obtained. The rate of convergence of the iterations are examined and the results compared with previous calculations.

1. Introduction. The Thomas-Fermi function, $\phi(x)$, for neutral atoms with spherical symmetry satisfies the non-linear second order differential equation

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

subject to the boundary conditions

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

(see [5]). From these conditions we may deduce that $\phi(x)$ belongs to the real Hilbert space where

$$\langle \psi_1 | \psi_2 \rangle = \int_0^\infty x e^{-x} \psi_1(x) \psi_2(x)\, dx \tag{3}$$

and

$$\langle \psi_1 | \psi_1 \rangle < \infty. \tag{4}$$

The operator

$$T = -xd^2/dx^2 - (2 - x)d/dx + 1 \tag{5}$$

is self-adjoint on a dense subspace $D(T)$ of this Hilbert space so that re-arranging (1) to

$$-xd^2\phi/dx^2 - (2 - x)\, d\phi/dx + \phi = -\phi^{3/2}x^{1/2} - (2 - x)\, d\phi/dx + \phi \tag{6}$$

we have an equation of the form

$$T\phi = f(\phi). \tag{7}$$

The variational-iterative theory given in [2, 3] and [4] can be used to obtain an approximate solution to this equation. For a given set of trial functions this approximate solution ψ satisfies

$$\delta J = 0 \quad \text{when } \psi = \psi_0 \tag{8}$$

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where

$$J(\psi, \psi_0) = \langle \psi | T\psi \rangle - 2\langle \psi | f(\psi_0) \rangle \tag{9}$$

and consequently

$$\delta J(\psi, \psi_0) = 2\langle \delta\psi | T\psi - f(\psi_0) \rangle. \tag{10}$$

2. The approximate solutions. A trial function for ϕ, $\psi = e^{-\beta x}$ ($\beta = 0.731745$) was previously found (see [2]) and in this note we extend the calculations by considering trial functions of the form

$$\psi = e^{-\beta x}\left(1 + \sum_{n=1}^{N} a_n x^n\right). \tag{11}$$

The results are given in the Table 1 for $N = 1, 2, 3, 4$ and 5 together with $\|T\psi - f(\psi)\|$ which provides a measure of convergence. These results for $N = 1$ and 5 are compared in Figs. 1, 2, 3 and 4 with those obtained by Anderson and Arthurs. They obtain two one-parameter function

$$\Phi = (1 + \gamma x^{1/2})e^{-\gamma x^{1/2}}; \tag{12}$$

$\gamma = 1.905$ and $\gamma = 1.750$ being their optimum values and obtained from separate maximum and minimum principles and

$$\Phi = (1 + \alpha x^{1/2} + \alpha^2 x/x)e^{-\alpha x^{1/2}} \tag{13}$$

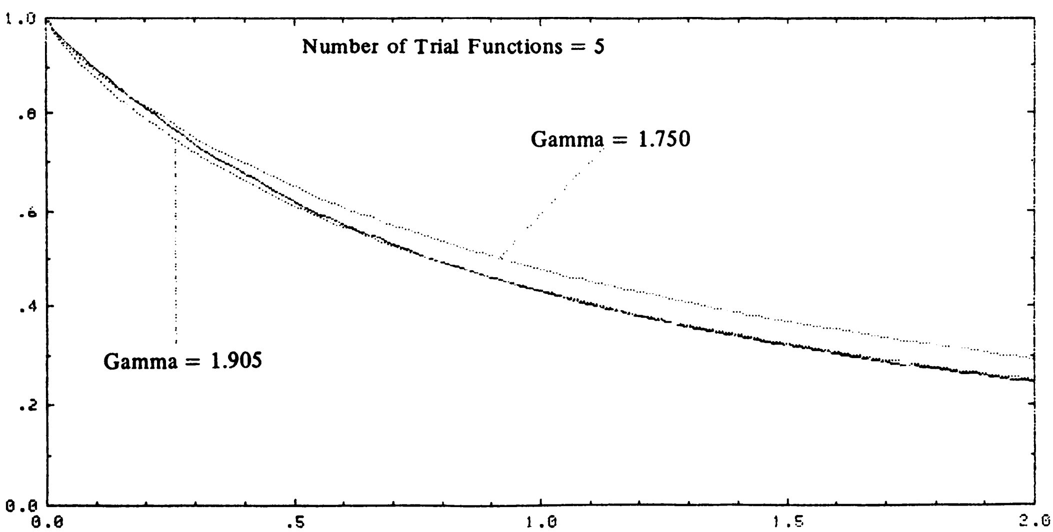

FIG. 1

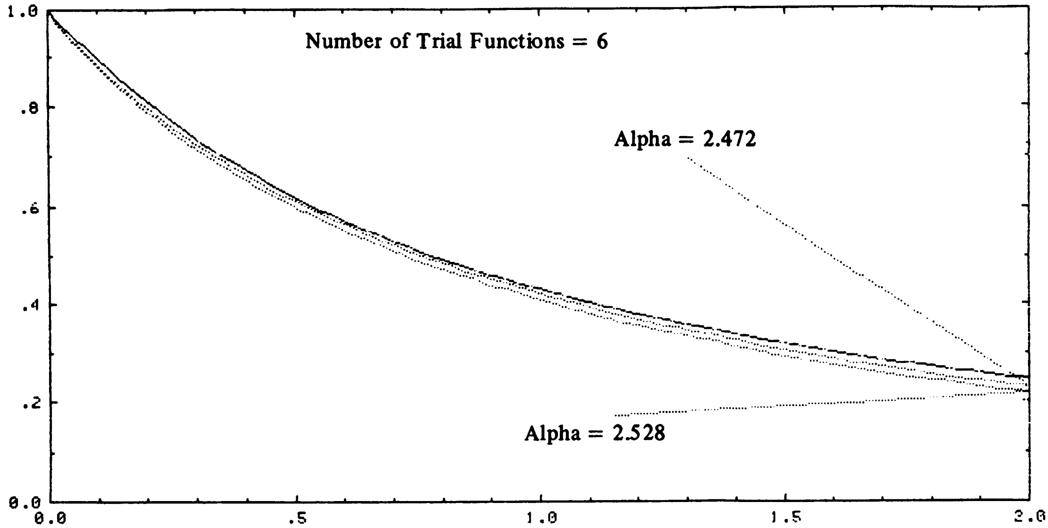

FIG. 2

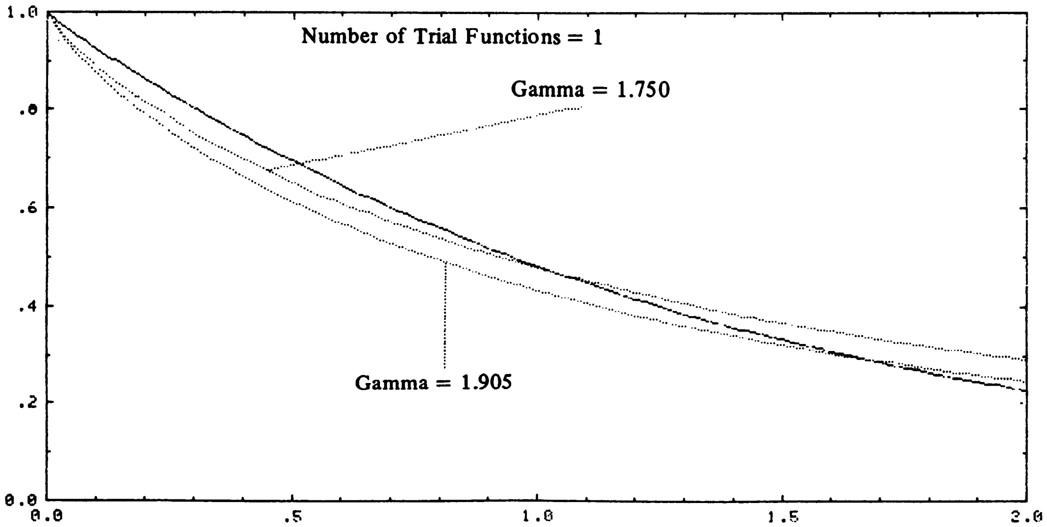

FIG. 3

with optimum values of $\alpha = 2.472$ and $\alpha = 2.528$. The simple form of our 1-parameter trial function which does not match the behaviour at the origin gives a worse result than Anderson and Arthurs whereas the 5-parameter function gives good agreement. The chief advantage of our form of trial function is that it can easily be extended by increasing N. We note that Eq. (15) of Anderson and Arthurs [1] is misprinted and the correct version is our Eq. (13).

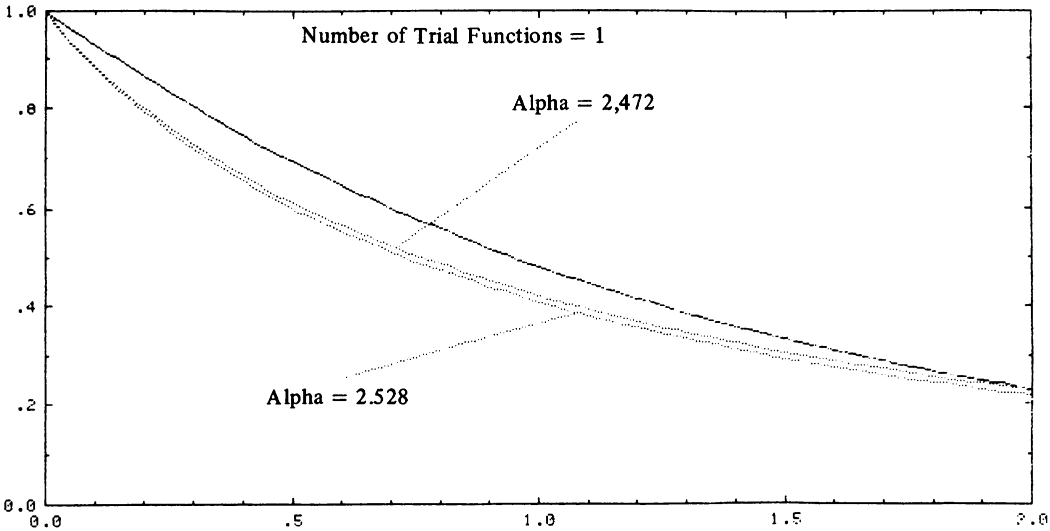

FIG. 4

TABLE 1

N	a_1	a_2	a_3	a_4	a_5	$\|T\psi - f(\psi)\|$
1	1.100×10^{-6}	–	–	–	–	1.208×10^{-1}
2	-2.017×10^{-1}	1.230×10^{-1}	–	–	–	4.707×10^{-2}
3	-2.545×10^{-1}	1.772×10^{-1}	-1.547×10^{-2}	–	–	3.830×10^{-2}
4	-3.256×10^{-1}	2.864×10^{-1}	-6.942×10^{-2}	8.792×10^{-3}	–	2.542×10^{-2}
5	-3.683×10^{-1}	3.689×10^{-1}	-1.295×10^{-1}	2.626×10^{-2}	-1.842×10^{-3}	1.992×10^{-2}

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