Thomas-Fermi Model

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The boundary value problem

$$y''(x) = x^{-1/2} y(x)^{3/2}, \qquad y(0) = 1, \qquad \lim_{x \to \infty} y(x) = 0$$

is an important model in atomic physics [1, 2, 3, 4]. Two well-known series expansions for $y(x)$ are

$$y(x) = \sum_{k=0}^{\infty} p_k x^{k/2}, \qquad x \approx 0$$

$$p_0 = 1, \qquad p_1 = 0, \qquad p_2 = -\xi, \qquad p_3 = 4/3, \qquad p_4 = 0, \qquad \ldots$$

due to Baker [5] and

$$y(x) = \frac{144}{x^3} \sum_{k=0}^{\infty} q_k \eta^k x^{-\lambda k}, \qquad x \approx \infty$$

$$q_0 = 1, \qquad q_1 = -1, \qquad \ldots$$

due to Coulson & March [6], where $\lambda = (-7 + \sqrt{73})/2$. The coefficient p_k is a polynomial in ξ; the coefficient $q_k \eta^k$ is (even more clearly) a polynomial in η. Hence it is important to compute

$$\xi = \lim_{x \to 0^+} \frac{1 - y(x)}{x} = -y'(0), \qquad \eta = \lim_{x \to \infty} x^{\lambda} \left(1 - \frac{x^3}{144} y(x) \right)$$

as accurately as feasible.

More precisely, we have recursive formulas [7, 8, 9]

$$\begin{aligned} p_k \;\; = \;\; & \frac{1}{(k-3)\left[(k-1)^2 - 1\right]} \left\{ \frac{3}{2} \sum_{j=1}^{k-4} (j+1) \left[(k-j-2)^2 - 1 \right] p_{j+1} p_{k-j-1} \right. \\ & \left. - \sum_{j=0}^{k-6} (j+1) \left[(j+3)^2 - 1 \right] p_{j+4} p_{k-j-4} \right\} \end{aligned}$$

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for $k \geq 5$ and

$$\begin{aligned} q_k \;=\; & \frac{1}{(k-1)k(\lambda^2 k+6)}\sum_{j=0}^{k-2}(j+1)\left\{\frac{3}{2}\left[\lambda^2(k-j-1)(k-j-2)\right.\right. \\ & \left.\left.+6(k-j-1)+12\right]-\lambda^2 j(j+1)-6(j+1)-12\right\} q_{j+1}q_{k-j-1} \end{aligned}$$

for $k \geq 2$. Special values include

$$p_5 = -\frac{2}{5}\xi, \qquad p_6 = \frac{1}{3}, \qquad p_7 = \frac{3}{70}\xi^2,$$

$$p_8 = -\frac{2}{15}\xi, \qquad p_9 = \frac{4}{63}\left(\frac{7}{6}+\frac{1}{16}\xi^3\right), \qquad p_{10} = \frac{1}{175}\xi^2$$

and

$$q_2 = \frac{201+21\sqrt{73}}{608}, \qquad q_3 = -\frac{15377+1813\sqrt{73}}{98496}.$$

Such information, however, does not lead easily to numerical estimates of ξ or η. Various attempts to do this include [10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29]. We mention that the solution $y(x)$ minimizes the integral

$$I(\varphi) = \int_0^\infty \left(\frac{1}{2}\varphi'(x)^2 + \frac{2}{5}\frac{\varphi(x)^{5/2}}{x^{1/2}}\right)dx$$

subject to the constraints $\varphi(0) = 1$ and $\lim_{x\to\infty}\varphi(x) = 0$, and maximizes the integral

$$J(\psi) = -\int_0^\infty \left(\frac{1}{2}\psi'(x)^2 + \frac{3}{5}\frac{(x^{1/2}\psi''(x))^{5/3}}{x^{1/2}}\right)dx - \psi'(0)$$

with no essential constraints [30, 31, 32]. The extreme values of I and J agree:

$$J(\psi) \leq J(y) = I(y) \leq I(\varphi)$$

and thus the difference $I(z) - J(z)$ serves to measure how close a candidate function $z(x)$ is to $y(x)$.

0.1. Majorana Transformation. The following derivation of ξ, η was discovered in 1928 but remained unknown until recently [33, 34]. Write

$$t = 144^{-1/6}x^{1/2}y(x)^{1/6},$$

$$u = -\left(\frac{16}{3}\right)^{1/3} y(x)^{-4/3}y'(x)$$

then

$$\dot{u}(t) = 8\frac{t\,u(t)^2 - 1}{1 - t^2 u(t)}, \qquad u(0) = \left(\frac{16}{3}\right)^{1/3}\xi, \qquad u(1) = 1$$

and hence

$$u(t) = \sum_{m=0}^{\infty} a_m (1-t)^m$$

where $a_0 = 1$, $a_1 = 9 - \sqrt{73}$ and

$$\begin{aligned} a_m &= \frac{1}{2(m+8)-(m+1)a_1}\left\{\sum_{n=1}^{m-2}\left[(n+1)a_{n+1} - 2(n+4)a_n + (n+7)a_{n-1}\right]a_{m-n}\right. \\ &\quad \left. + \left[(m+7) - 2(m+3)a_1\right]a_{m-1} + (m+6)a_1 a_{m-2}\right\}. \end{aligned}$$

It follows that

$$\xi = \left(\frac{3}{16}\right)^{1/3}\sum_{m=0}^{\infty} a_m = 1.5880710226....$$

We have

$$y(x) = \frac{144}{x^3}t^6,$$

$$x(t) = 144^{1/3}t^2 \exp\left[2\int_0^t \frac{s\,u(s)}{1-s^2u(s)}ds\right]$$

and, further,

$$\int_0^t \frac{s\,u(s)}{1-s^2u(s)}ds = \int_{1-t}^1 \frac{\sum_{m=0}^{\infty} b_m \tau^m}{\sum_{m=0}^{\infty} c_m \tau^m}d\tau$$

where $b_0 = 1$, $c_0 = 0$,

$$b_m = a_m - a_{m-1}, \qquad c_m = b_{m-1} - b_m \qquad \text{for } m \geq 1.$$

It follows that

$$\eta = \lim_{t \to 1^-} x(t)^{\lambda}\left(1 - t^6\right) = 13.2709738480....$$

These numerical computations appear to be more straightforward than any other technique invented over the past eighty years!

A starting point for theory underlying the Thomas-Fermi equation can be found in [35, 36, 37, 38]; see also [39] for a connection with counting lattice points within a planar closed curve.

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