PHYSICAL REVIEW A VOLUME 45, NUMBER 1 1 JANUARY 1992

Thomas-Fermi-Scott model in momentum space

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(Received 10 May 1991)

We incorporate the Scott correction into the momentum-space energy functional of the Thomas-Fermi model and so improve the description of the strongly bound electrons. The resulting differential equation is then discussed, and we report numerical results for neutral mercury.

PACS number(s): 31.15.+q, 31.20.Sy, 31.20.Lr, 31.90.+s

INTRODUCTION

"The well-known failure of the Thomas-Fermi (TF) model in the vicinity of the atomic nucleus requires a special treatment of the strongly bound electrons. This is generally called the Scott correction [1]. It can be incorporated consistently into the TF model, provided the language of potential functionals is employed [2]. Thus one arrives at the Thomas-Fermi-Scott (TFS) model. All physical quantities, for which the contribution from the innermost electrons is dominating or at least substantial, are treated much more realistically in the TFS model than in the TF model." So begins a recent paper [3] on the Scott correction to the momental density. It is the objective of the present contribution to present the momentum-space formulation of the TFS model, thereby improving upon the TF approximation reported in the preceding paper (I) [4].

MOMENTAL TFS MODEL

The reasoning that produced the spatial TFS energy functional in Chap. 3 of Ref. [5] can be repeated for the $\tilde{E}_1[T+\zeta]$ given in Eq. (41) of I. This leads to

$$\tilde{E}_1^{\mathrm{TFS}}[T+\zeta]=\tilde{E}_1^{\mathrm{TF}}[T+\zeta]+\Delta_S\tilde{E}_1[T+\zeta] \tag{1}$$

with the Scott correction

$$\Delta_S\tilde{E}_1[T+\zeta]=\left\{\zeta N_s-2Z^2[\nu_s]+\int(d\mathbf{p}')T(\mathbf{p}')\sum_{\nu=1}^{[\nu_s]}2\nu^2|\psi_\nu|^2_{\mathrm{av}}(p')-\left[1-(\zeta_s-\zeta)\frac{\partial}{\partial\zeta_s}\right]\tilde{E}_1^{\mathrm{TF}}[T+\zeta_s]\right\}_{\mathrm{SP}} . \tag{2}$$

Here, $|\psi_\nu|^2_{\mathrm{av}}(p')$ is the average momental density of one electron in the νth Bohr shell, explicitly given by [6]

$$|\psi_\nu|^2_{\mathrm{av}}(p')=\frac{8}{\pi^2}\frac{(\nu/Z)^3}{[1+(\nu p'/Z)^2]^4} ; \tag{3}$$

ν_s plays the role of a continuous principal quantum number; the binding energy ζ_s that separates the specially treated strongly bound electrons from the other ones is related to $T(\mathbf{p}')$ and ν_s by

$$\zeta_s=\frac{Z^2}{2\nu_s^2}-\int(d\mathbf{p}')[T(\mathbf{p}')-\tfrac{1}{2}p'^2]|\psi_{\nu_s}|^2_{\mathrm{av}}(p') ; \tag{4}$$

and the number N_s of strongly bound electrons is

$$N_s=\sum_{\nu=1}^{[\nu_s]}2n^2=\tfrac{2}{3}[\nu_s]([\nu_s]+\tfrac{1}{2})([\nu_s]+1) . \tag{5}$$

The curly brackets $\{f(\nu_s)\}_{\mathrm{SP}}$ in Eq. (2) symbolize the injunction to evaluate the *smooth part* of this function of ν_s, thereby discarding all oscillatory contributions that arise because some terms involve the integer part $[\nu_s]$ of ν_s.

The various smooth parts are [5]

$$\{[\nu_s]\}_{\mathrm{SP}}=\nu_s-\tfrac{1}{2} , \quad \{N_s\}_{\mathrm{SP}}=\tfrac{2}{3}\nu_s^3 , \tag{6}$$

and [3]

$$\left\{\sum_{\nu=1}^{[\nu_s]}2\nu^2|\psi_\nu|^2_{\mathrm{av}}(p')\right\}_{\mathrm{SP}}=\Delta_S\rho(p')+\frac{1}{3\pi^2}\left[\frac{2\nu_s^2/Z}{1+(\nu_s p'/Z)^2}\right]^3 \tag{7}$$

with

$$\begin{aligned}\Delta_S\rho(p')&=\left[\frac{4Z}{\pi}\right]^2\sum_{\nu=1}^{\infty}\frac{(\nu/Z)^5}{[1+(\nu p'/Z)^2]^4}-\frac{1}{3\pi^2}\left[\frac{2Z}{p'^2}\right]^3\\&=-\frac{1}{3\pi^2}\left[\frac{Z}{p'}\frac{\partial}{\partial p'}\right]^3[\mathrm{Re}\varphi(iZ/p')+\ln(p'/Z)] ,\end{aligned} \tag{8}$$

where the latter version involves the logarithmic derivative of the factorial function: $\varphi(x)=d\ln(x!)/dx$. Consequently, the Scott correction (2) is

$$\begin{aligned}\Delta_S\widetilde{E}_1=&\tfrac{1}{2}Z^2+\int(d\mathbf{p}')[T(\mathbf{p}')-\tfrac{1}{2}p'^2+\zeta]\Delta_S\rho(p')\\&-Z^2\nu_s+\int(d\mathbf{p}')[T(\mathbf{p}')-\tfrac{1}{2}p'^2+\zeta]\\&\times\frac{1}{3\pi^2}\left[\frac{2\nu_s^2/Z}{1+(\nu_s p'/Z)^2}\right]^3\\&-\left[1-(\zeta_s-\zeta)\frac{\partial}{\partial\zeta_s}\right]\widetilde{E}_1^{\mathrm{TF}}[T+\zeta_s]\ ,\end{aligned}\tag{9}$$

where the identities

$$\begin{aligned}&\int(d\mathbf{p}')\Delta_S\rho(p')=0\ ,\\&\int(d\mathbf{p}')\Delta_S\rho(p')\tfrac{1}{2}p'^2=-\tfrac{1}{2}Z^2\ ,\\&\int(d\mathbf{p}')\frac{1}{3\pi^2}\left[\frac{2\nu_s^2/Z}{1+(\nu_s p'/Z)^2}\right]^3=\tfrac{2}{3}\nu_s^3\ ,\\&\int(d\mathbf{p}')\frac{1}{3\pi^2}\left[\frac{2\nu_s^2/Z}{1+(\nu_s p'/Z)^2}\right]^3\tfrac{1}{2}p'^2=Z\nu_s^2\end{aligned}\tag{10}$$

have been used for regrouping the terms. The first two contributions to $\Delta_S\widetilde{E}_1$ in (9) are independent of ν_s, whereas the other three do depend on this parameter. This dependence, however, is only apparent. For, since ζ_s is large on the TF scale of energies and small on the Bohr scale, [1,2,5]

$$Z^{4/3}\ll\zeta_s\ll Z^2\ ,\tag{11}$$

and because the main contribution to the last two terms on the right-hand side (rhs) of (9) comes from p' values around $p'\sim Z/\nu_s\cong\sqrt{2\zeta_s}\gg Z^{2/3}$, these terms are—not unexpectedly—significant only for strongly bound electrons. For those, the effective kinetic energy $T(\mathbf{p}')$ differs from $T_{\mathrm{kin}}=\frac{1}{2}p'^2$ by an additive constant,

$$T(\mathbf{p}')\cong\tfrac{1}{2}p'^2+C\ ,\tag{12}$$

with C related to the energy as in Eq. (67) of I. Then (4) implies

$$\zeta_s\cong\frac{Z^2}{2\nu_s^2}-C\ ,\tag{13}$$

and

$$T(\mathbf{p}')+\zeta_s\cong\tfrac{1}{2}p'^2+\frac{Z^2}{2\nu_s^2}=\frac{1}{2}\left[\frac{Z}{\nu_s}\right]^2[1+(\nu_s p'/Z)^2]\tag{14}$$

produces

$$\left[1-(\zeta_s-\zeta)\frac{\partial}{\partial\zeta_s}\right]\widetilde{E}_1^{\mathrm{TF}}[T+\zeta_s]\cong-\tfrac{2}{3}Z^2\nu_s-\tfrac{2}{3}\nu_s^3(\zeta_s-\zeta)\tag{15}$$

as well as

$$\int(d\mathbf{p}')[T(\mathbf{p}')-\tfrac{1}{2}p'^2+\zeta]\frac{1}{3\pi^2}\left[\frac{2\nu_s^2/Z}{1+(\nu_s p'/Z)^2}\right]^3\cong\tfrac{1}{3}Z^2\nu_s-\tfrac{2}{3}\nu_s^3(\zeta_s-\zeta)\ ,\tag{16}$$

so that the ν_s-dependent terms in (9) compensate for each other exactly, where they are relevant. This leaves us with

$$\Delta_S\widetilde{E}_1[T+\zeta]=\tfrac{1}{2}Z^2+\int(d\mathbf{p}')[T(\mathbf{p}')-\tfrac{1}{2}p'^2+\zeta]\Delta_S\rho(p')\ .\tag{17}$$

In view of (10), the contribution proportional to ζ equals zero, but we prefer to include it anyway in order to emphasize that $\Delta_S\widetilde{E}_1$ is a functional of the sum $T+\zeta$ as it should be. The perturbative evaluation of $\Delta_S\widetilde{E}_1$, achieved by inserting (12) into (17), reproduces the well-known [1] Scott correction of $\frac{1}{2}Z^2$ to the actual energy of the atom,

$$E^{\mathrm{TFS}}(Z,N)=E^{\mathrm{TF}}(Z,N)+\tfrac{1}{2}Z^2\ .\tag{18}$$

As is typical for a Scott correction, it is the same for all degrees of ionization.

When the Scott correction is added to the TF functional given in Eq. (60) of I, we arrive at the momental TFS functional,

$$\begin{aligned}\widetilde{E}^{\mathrm{TFS}}[T,\rho,\zeta]=&\tfrac{1}{2}Z^2+\int(d\mathbf{p}')\left[-\frac{Z^3}{6\pi^2}\right][T(\mathbf{p}')+\zeta]^{-2}-\int(d\mathbf{p}')[T(\mathbf{p}')-\tfrac{1}{2}p'^2][\rho(\mathbf{p}')-\Delta_S\rho(p')]\\&+\tfrac{3}{4}(3\pi^2)^{-1/3}\int(d\mathbf{p}')(d\mathbf{p}'')(\rho_>^{2/3}\rho_<-\tfrac{1}{5}\rho_<^{5/3})-\zeta N\ .\end{aligned}\tag{19}$$

The stationary property under variations of $T(\mathbf{p}')$ implies

$$\rho(\mathbf{p}')=\frac{Z^3}{3\pi^2}[T(\mathbf{p}')+\zeta]^{-3}+\Delta_S\rho(p')\ ,\tag{20}$$

which replaces the TF relation in (50) of I, and variations of $\rho(\mathbf{p}')$ and ζ reproduce (64) and (30) of I. We can solve (20) for $T+\zeta$, use this expression in (19), and find the TFS approximation to $\widetilde{E}_{\mathrm{ext}}[\rho]$,

$$\begin{aligned}\widetilde{E}_{\mathrm{ext}}^{\mathrm{TFS}}[\rho]&=Z^2+\int(d\mathbf{p}')\left[-\frac{Z}{2\pi^2}\right]\\&\qquad\times\{3\pi^2[\rho(\mathbf{p}')-\Delta_S\rho(p')]\}^{2/3}\\&=Z^2+\widetilde{E}_{\mathrm{ext}}^{\mathrm{TF}}[\rho-\Delta_S\rho]\ .\end{aligned}\tag{21}$$

This functional equals the ground-state expectation value of H_{ext}, see (29b) of I, and should therefore be linear in the atomic number Z. The intrinsic Z dependence of $\Delta_S\rho$ and the additive constant Z^2 are, however, of higher order in Z. These Z dependences must be regarded as implicit, because they originate in the hydrogenic wave functions that were used in the derivation of (17) and (21). So the TFS functionals apply to $T_{\mathrm{kin}}(p)=\frac{1}{2}p^2$ only; the structures of (17) and (21) are not universal in the sense that they can be used for any T_{kin}. We need to keep this in mind to not run into inconsistencies [7]. For example, when invoking the stationary property of the energy functional to derive

$$T(\mathbf{p}')-\tfrac{1}{2}p'^2 \rightarrow -\frac{\partial}{\partial Z}E^{\mathrm{TFS}}(Z,N) \quad \text{as } p'\rightarrow\infty \tag{22}$$

in analogy to (66) of I, only the explicit Z dependence of $\tilde{E}^{\mathrm{TFS}}_{\mathrm{ext}}$ must be taken into account.

In conjunction with $\zeta=-\partial E^{\mathrm{TFS}}(Z,N)/\partial N$ and [3]

$$\Delta_S\rho(p')=-\frac{1}{3\pi^2}\left(\frac{2Z}{p'^2}\right)^3+\left(\frac{4}{\pi}\right)^2\frac{Z^5}{p'^8}\zeta_R(3)+\cdots\ , \tag{23}$$

where $\zeta_R(z)$ is the Riemann zeta function, Eqs. (20) and (22) reproduce Eq. (11) of Ref. [3],

$$\rho(p')=\frac{8}{\pi}n_0\frac{Z^2}{p'^8}+\cdots\ . \tag{24}$$

Here, n_0 denotes the spatial TFS density at the site of the nucleus,

$$n_0=\frac{(2Z)^3}{4\pi}\left[\zeta_R(3)+\frac{1}{Z^2}\left(\frac{\partial}{\partial Z}+\frac{\partial}{\partial N}\right)E^{\mathrm{TFS}}(Z,N)\right]\ , \tag{25}$$

and the ellipses indicate terms of order p'^{-10}. Note, in particular, that the two p'^{-6} terms in (20) cancel each other. More details about $\Delta_S\rho(p')$ and TFS expectation values of momentum functions are reported in Ref. [3].

When the transition from the TF model to the TFS model is made either in configuration space or in momentum space, the same physical ideas enter. Nevertheless, the TFS model defined by the momental functional (19) is not identical to the model based on the spatial functional of Refs. [2] or [5]. Of course, where the TFS approximation is reliable, the predictions of the two versions must agree. But the perfect equivalence, that was found for the TF models in I, cannot be expected for the two TFS variants.

It is remarkable that the spatial TFS energy functional [2,5] could not be brought into as compact a form as (19), because the spatial analog of (7) is not available as yet. Therefore, it was not possible to extract the smooth part from the spatial analog of (2) explicitly, and the discarding of the oscillatory terms had to be left as an injunction, which can be realized in a numerical scheme by averaging over a suitable range of ν_s values. Matters are much simpler in momentum space in this regard, since the average momental density (3) is a rather elementary function of the quantum number ν, whereas the average spatial density possesses a comparably complicated ν dependence, which could not be extended to noninteger values of ν as yet.

DIFFERENTIAL EQUATION

The TFS set of equations, namely (30) and (64) of I supplemented by (20), is more conveniently handled after rewriting the integral equations in terms of an equivalent differential equation with appropriate boundary conditions. The change of variables that was useful in transforming (64) of I into (73) of I suggests the following parametrizations:

$$\begin{aligned}
&[3\pi^3\rho(\mathbf{p}')]^{1/3}=R'=Z^{-1/3}ax\ ,\\
&T(p')+\zeta-\tfrac{1}{2}\mathbf{p}'^2=\frac{Z}{R'}[1-f(x)]\ ,\\
&\tfrac{1}{2}p'^2=\frac{Z^{4/3}}{a}[y(x)]^2
\end{aligned} \tag{26}$$

with $a=\frac{1}{2}(3\pi/4)^{2/3}=0.8853$, a constant familiar in the TF model. The various powers of Z in (26) are chosen in accordance with the Z dependences known from the TF model, and (26) follows, of course, the TF pattern quite deliberately. Before proceeding, we observe that the R' range $0\le R'\le R_0$ corresponds to $0\le x\le x_0$ and $\infty\ge y\ge 0$. The situation $x_0=\infty$ is possible and, indeed, realized for neutral TFS atoms. Equation (68) of I, which remains valid, then relates the value of the function $f(x)$ at the boundary $x=x_0$ to ζ,

$$\zeta=\frac{Z^{4/3}}{a}\frac{q-f(x_0)}{x_0}\ , \tag{27}$$

where $q=1-N/Z$ is the degree of ionization. The value of ζ must not be negative, so that $f(x_0)\le q$ is implied.

Next we insert (26) and (27) into (64) of I and arrive at

$$\begin{aligned}
f(x)=1&-\frac{x}{x_0}[q-f(x_0)]\\
&-\int_0^{x_0}dx'x'\min(x,x')[y(x')]^3\ ,
\end{aligned} \tag{28}$$

which has the consequences

$$f(x_0)-x_0f'(x_0)=q \tag{29}$$

$[f'(x)=df(x)/dx]$ and

$$\left(\frac{d}{dx}\right)^2 f(x)=f''(x)=x[y(x)]^3\ . \tag{30}$$

Note that for $y(x)=\sqrt{f(x)/x}$ this is the well-known TF equation. In the TFS model, however, the relation between $y(x)$, x, and $f(x)$ is different. It is given by Eq. (20), which now appears as

$$f(x)=1+x[y(x)]^2-\left(1-\frac{h(w)}{Z^2x^3}\right)^{-1/3} \tag{31}$$

with

$$w=(p'/Z)^2=\frac{2}{a}Z^{-2/3}[y(x)]^2 \tag{32}$$

and

$$\begin{aligned}
h(w)&=3\pi^2(Z/a)^3\Delta_S\rho(p')\\
&=(2/a)^3\left(6\sum_{\nu=1}^{\infty}\frac{\nu^5}{(1+\nu^2w)^4}-\frac{1}{w^3}\right)\\
&=-\left(\frac{2}{a}\frac{d}{dw}\right)^3[\mathrm{Re}\varphi(i/\sqrt{w})+\ln\sqrt{w}\,]\ .
\end{aligned} \tag{33}$$

In view of $y(x_0)=0$ and $h(0)=-4/(21a^3)$, we learn from (31) that

$$\begin{aligned}
f(x_0)&=1-\left(1-\frac{h(0)}{Z^2x_0^3}\right)^{-1/3}\\
&=1-\left(1+\frac{4/21}{Z^2(ax_0)^3}\right)^{-1/3}\ ,
\end{aligned} \tag{34}$$

so that $f(x_0)\ge 0$. Together with the inequality implied by (27), we thus have

$$0 \leq f(x_0) \leq q \ . \tag{35}$$

For neutral TFS atoms, when $N=Z$ and $q=0$, this says $f(x_0)=0$, and then Eq. (34) requires $x_0=\infty$. After supplementing Eqs. (29)–(31) and (34) with the boundary condition at $x=0$,

$$f(0)=1 \ , \tag{36}$$

as implied by (28), we have succeeded in writing the momental TFS equations as a differential equation with boundary conditions.

The new differential equation differs from the corresponding TF equation by the presence of the $h(w)$ terms in (31) and (34). Indeed, for $h(w)\equiv 0$, we return to the TF model. Also, the momental TFS differential equation—(30) with $y(x)$ determined by (31)—is not equivalent to the Poisson equation obeyed by the effective potential in the spatial TFS model [2,5]. This observation illustrates the remark, made in the paragraph after Eq. (25), that the spatial and the momental version of the TFS model are not identical.

The $h(w)$ terms in (31) and (34) are most important, naturally, for large momenta, which is to say for small values of x. The qualitative statement that $y\longrightarrow\infty$ as $x\longrightarrow 0$ is quantified by Eq. (24),

$$x^3 y^8 \longrightarrow \frac{3\pi}{2} a Z^{-7/3} n_0 \quad \text{for } x\longrightarrow 0 \ . \tag{37}$$

Combined with the large-w form of $h(w)$, see Eq. (23),

$$h(w)=\left[\frac{2}{a}\right]^3 \left[-\frac{1}{w^3}+\frac{6\zeta_R(3)}{w^4}+\cdots\right] , \tag{38}$$

this produces

$$-f'(0)=a\zeta_R(3)Z^{2/3}-\frac{\pi}{2}aZ^{-7/3}n_0 \tag{39}$$

when used in (31). In view of (25),

$$-f'(0)\cong -aZ^{-4/3}\left[\frac{\partial}{\partial Z}+\frac{\partial}{\partial N}\right]E^{\text{TFS}}(Z,N) \tag{40}$$

can be expected to hold with high accuracy. In particular, for neutral atoms this reads

$$-f'(0)\cong B-aZ^{-1/3} \ , \tag{41}$$

where $B=1.588\,071$ is Baker's constant [8], the initial slope of the neutral-atom TF function. Another consequence of (37) is

$$f''(x)\cong\left[\frac{3\pi}{2}aZ^{-7/3}n_0\right]^{3/8} x^{-1/8} \quad \text{for } x \gtrsim 0 \ , \tag{42}$$

so that

$$\begin{aligned} f(x) &\cong 1+f'(0)x+\frac{64}{105}\left[\frac{3\pi}{2}aZ^{-7/3}n_0\right]^{3/8} x^{15/8} \\ &= 1+f'(0)x \\ &\quad +\tfrac{64}{105}[3a\zeta_R(3)Z^{2/3}+3f'(0)]^{3/8}x^{15/8} \end{aligned} \tag{43}$$

for sufficiently small values of x. This is markedly different from the TF function, for which the first term beyond the linear one is $\frac{4}{3}x^{3/2}$.

For small momenta, thus large values of x, the effect of the $h(w)$ terms in (31) and (34) is negligible to a large extent. For instance, the asymptotic form of $f(x)$ for neutral atoms is given by

$$\begin{aligned} f(x) &= \frac{144}{x^3}(1+\epsilon)(1-\beta x^{-\gamma}+\cdots) \ , \\ \gamma &= \tfrac{1}{2}[-7+\sqrt{1+72(1+\epsilon)^{1/3}}\,] \ , \end{aligned} \tag{44}$$

where the constant β is very close to its TF value of 13.270 974, and the deviation of ϵ from the TF limit ($\epsilon=0$) is found by solving

$$1+\epsilon=(1+\epsilon)^{2/3}+\tfrac{1}{3}(Z_0/Z)^2 \tag{45}$$

with $Z_0=\frac{1}{12}\sqrt{-h(0)}=0.0437$. Since $(Z_0/Z)^2 \ll 1$ is always true, this yields

$$\epsilon\cong (Z_0/Z)^2 \ , \tag{46}$$

which is indeed very small.

NUMERICAL RESULTS

We have solved the new differential equation numerically for neutral mercury ($Z=N=80$). This was done be integrating (30) both from $x=0$ on outwards, and inwards from $x=\infty$, whereby the appropriate power series, of which the leading terms are given in (43) and (44), were used to get away from the singularities at the boundaries. The values of the respective parameters—the limit of (37) for the small-x expansion, and β of (44) for the large-x one—were then determined by matching both $f(x)$ and $f'(x)$ at an intermediate point. The resulting numbers are

$$\frac{3\pi}{2}aZ^{-7/3}n_0=54.904\,994\,455 \tag{47}$$

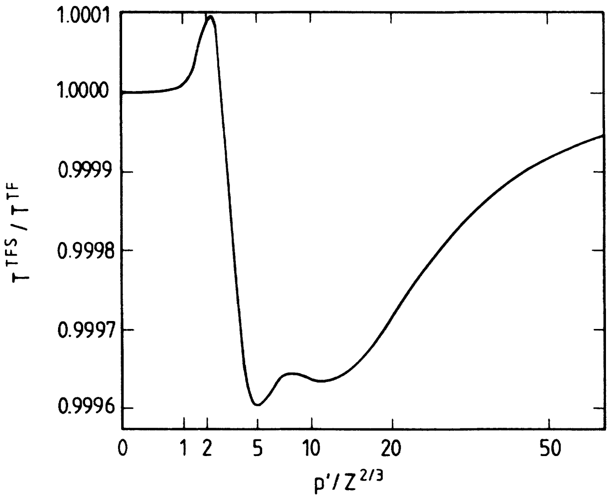

FIG. 1. Ratio of effective kinetic energies, $T^{\text{TFS}}/T^{\text{TF}}$, as a function of p', for neutral mercury. The abscissa is linear in the square root of p'.

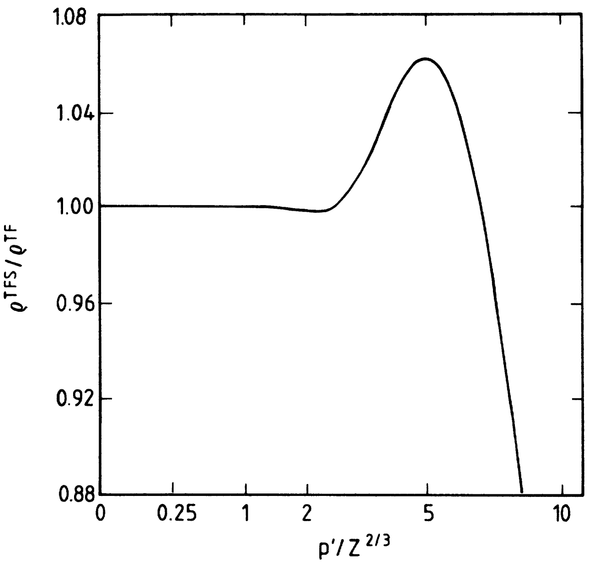

FIG. 2. Ratio of the momental densities, $\rho^{\mathrm{TFS}}/\rho^{\mathrm{TF}}$, as a function of p', for neutral mercury. The abscissa is linear in the square root of p'.

and

$$\beta = 13.270\,952\,872\ ; \tag{48}$$

the eleven digits reported here are not sensitive to the details of the numerical procedure. It is reassuring that β agrees with the corresponding TF value to one part in a million, and the perturbative estimate [Eqs. (39) and (41)]

$$\begin{aligned} n_0 \Big/ \frac{(2Z)^3}{4\pi} &= \zeta_R(3) - \frac{B}{a} Z^{-2/3} + \frac{1}{Z} \\ &= 1.117\,945 \text{ for } Z = 80\ , \end{aligned} \tag{49}$$

is only 0.4% larger than the actual value of 1.113 405 computed from (47).

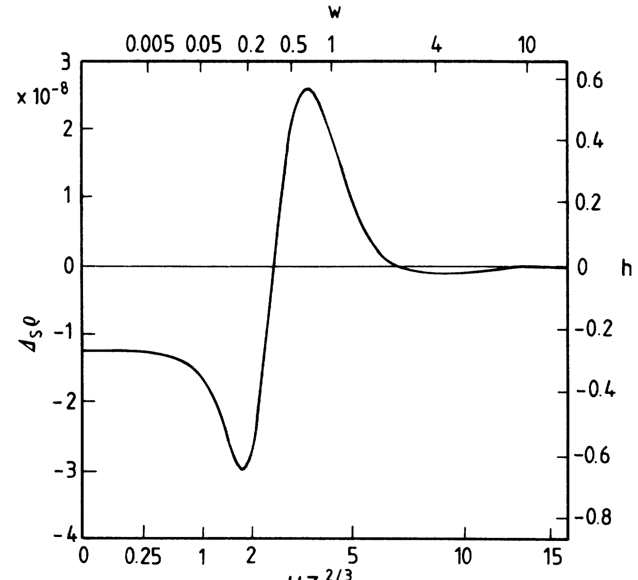

FIG. 3. The Scott correction $\Delta_S\rho$ as a function of p', for mercury. The abscissa is linear in the square root of p'. Inasmuch as $h = \frac{128}{3} Z^3 \Delta_S \rho(p')$ is a Z-independent function of $w = (p'/Z)^2$, the plot is readily applied to different values of Z.

The radial momental density and the effective kinetic energy in the neutral mercury atom are indiscernible from the results for the TF quantities that are plotted in Fig. 1 of I. The effect of the Scott correction is evident in Figs. 1 and 2 which present the ratios $T^{\mathrm{TFS}}/T^{\mathrm{TF}}$ and $\rho^{\mathrm{TFS}}/\rho^{\mathrm{TF}}$. Please note that the ratio of the effective kinetic energies is very close to unity, much closer indeed than the ratio $V^{\mathrm{TFS}}/V^{\mathrm{TF}}$ of the effective potentials [see Fig. 3-7 in Ref. [5]). In contrast, for $p'/Z^{2/3} \gtrsim 2$ or $p' \gtrsim 40$, the difference between the TFS and the TF density is substantial, as is visible in Fig. 2. (In Fig. 1 of I this p' range is not covered.)

For completeness, we give a plot of $\Delta_S\rho$ in Fig. 3. Please observe that $\Delta_S\rho$ is of small magnitude, and it is negative save for the range [9] $0.588\,413 < p'/Z < 1.558\,281$, that is $2.535 < p'/Z^{2/3} < 6.714$ for $Z = 80$.

ACKNOWLEDGMENTS

B.G.E. expresses his gratitude for the kind hospitality experienced at the Institute of Physical Chemistry and thanks Professor Olszewski in particular.

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[1] J. M. S. Scott, Philos. Mag **43**, 859 (1952); J. Schwinger, Phys. Rev. A **22**, 1827 (1980).
[2] B.-G. Englert and J. Schwinger, Phys. Rev. A **29**, 2331 (1984); for a list of misprints in this paper see Ref. [5], p. 387.
[3] K. Buchwald and B.-G. Englert, Phys. Rev. A **40**, 2738 (1989).
[4] B.-G. Englert, preceding paper, Phys. Rev. A **44**, 127 (1991).
[5] B.-G. Englert, *Semiclassical Theory of Atoms,* Vol. 300 of *Lecture Notes in Physics,* edited by J. Ehlers *et al.* (Springer-Verlag, Berlin, 1988).
[6] An elegant, concise derivation of the hydrogenic wave functions in momentum space is given by J. Schwinger, J. Math. Phys. **5**, 1606 (1964).
[7] Compare with the related discussion concerning the spatial TFS functional in Ref. [5], pp. 148–155.
[8] E. Baker, Phys. Rev. **36**, 630 (1930).
[9] K. Buchwald, Diplomarbeit, Universität München, 1989.