Myron's Work on the Thomas-Fermi Atom Revisited

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In late 1990's I got interested in applying field theory methods to plasma physics. Wrote a wonderful Physics Report paper with Larry Yaffe which made zero impact. No plasma person has ever read it; they only vie with one another to have the largest code on the biggest computer.

So I continued doing plasma physics *a la* field theory.

In 2000, after many years, I graduated from Univ. Wash. Marshall Baker gave me Schwinger's Quantum Mechanics Book as a Graduation Present. I looked though it and found that the last chapter had a detailed account of the Thomas-Fermi atom to which I did not pay much attention.

Around 2005 I became interested in the problem of heavy impurity atoms in a plasma of light ions. I remembered Baker/Schwinger/Thomas-Fermi. I found that the problem could be described in field theory language if the impurity atoms were described by the Thomas-Fermi model. The problem could be easily solved for very dilute impurities — the atoms automatically ionized as the plasma was heated — not an ad-hoc artificial fixed ionization state, but a proper thermodynamical mixture emerged.

With this in hand, I thought that I could outdo Schwinger: Compute all known corrections to T-F as Schwinger had done in that chapter but using elegant and economical quantum field theory methods.

Thomas-Fermi atomic energy + known corrections:

$$-E = \left\{ \underbrace{C_{1/3}\, Z^{1/3}}_{\text{Std. T}-\text{F}} + \underbrace{C_0}_{\text{Short Dist. Q.M.}} + \underbrace{C_{-1/3}\, Z^{-1/3}}_{\text{Long Dist. Q.M.+Exch.}} \right\} \frac{Z^2\, e^2}{4\pi\, a_0}$$

$$a_0 = \text{Bohr} \quad \text{radius}$$

I also conjectured that no more perturbative terms in powers of $Z^{-1/3}$ could be computed — at higher orders one has run out of smoothness, and non-analytic atomic shell structure predominates.

I described this conjecture a few years ago to an audience — their eyes just glazed over.

Method

Work with very dilute gas of very cold atoms $\Leftrightarrow$ isolated atom. Compute energy E and electron number N_e per nuclear particle of charge Z using thermal quantum field theory functional integration techniques. $N_e = Z$ for neutral atom.

Introduce auxiliary scalar field coupled to the electron and nuclear charge densities with an additional Gaussian term so that completing the square and performing the scalar field functional integral gives back the original Coulomb interactions.

Reserve scalar field integration till last. Perform Fermi functional integrals to get Fredholm determinant factors. Take infinite nuclear mass limit so its Fredholm determinate gives trivial exponential contribution.

Resulting Expression For Atomic Binding Energy

$$e^{-\beta(E-\mu_e N_e)} =$$

$$\int [d\chi] \exp\left\{-\int_0^\beta d\tau \int (d^3\mathbf{r}) \left[\frac{1}{2}\Big(\nabla\chi(\mathbf{r},\tau)\Big)^2 - iZe\delta(\mathbf{r})\,\chi(\mathbf{r},\tau)\right]\right\}$$

$$\mathrm{Det}^2 \left[\frac{\partial}{\partial\tau} + \frac{-\nabla^2}{2m_e} - \mu_e + ie\chi(\mathbf{r},\tau)\right]$$

Take zero temperature limit $\beta = \frac{1}{T} \to \infty$

Calculate, Calculate, Calculate for 10 pages

Find Exact Atomic Binding Energy Formula

$$E - \mu_e N_e = \int (d^3\mathbf{r}) \left[-\frac{1}{2} \Big(\nabla \phi_{\rm cl}(\mathbf{r}) \Big)^2 + Ze\delta(\mathbf{r})\, \phi_{\rm cl}(\mathbf{r}) \right] + W_e[\phi_{\rm cl}]$$

$\phi_{\rm cl}$ solution of $\delta \left(E - \mu_e N_e \right) = 0$

$$W_e[\phi] = \underbrace{W_{e,0}[\phi]}_{\text{Hartree Approx.}} + \underbrace{W_{e,\neq 0}[\phi]}_{\text{Non}-\text{Zero Modes}}$$

Explicitly

$$W_{e,0}[\phi] = -2\,\mathrm{Tr}\left(\mu_e - \mathcal{H}\right)\, \theta\left(\mu_e - \mathcal{H}\right)$$

$W_{e,\neq 0}[\phi]$ = Result of functional integral over non-zero modes in electron Fredholm determinant $\Rightarrow$ Exchange Corrections

I recently discovered Myron's paper

Corrections to the Thomas-Fermi Model of the Atom
Annals of Physics **144**, 1-14 (1982)

Myron got essentially the result above in two pages (with the help of a little physical intuition)

I computed $C_{1/3}$, C_0, $C_{-1/3}$ in 18 more pages = 28 total.
Schwinger did it in 24 pages. (I lost)
Myron did it in $2 + 9 = 11$ pages. (He won)

How Was Myron So Quick?

1. He used a path integral to obtain the classical limit and the $\hbar^2$ corrections.
   (I used a cumbersome expansion of the Wigner function.)

2. He expressed the short-distance corrections that comprise C_0 in terms of a subtraction of the Coulomb potential to both the order 1 and order $\hbar^2$ correction so that he could make use of the resulting expression when he turned to compute the long-distance Q.M. corrections in $C_{-1/3}$.
   (I did separate calculations so did the same work twice.)

3. He just omitted some intermediate steps in computing the exchange energy contribution to $C_{-1/3}$!

MY (???) CONJECTURE

I have already said that, in a talk to an audience of glazed eyes, I claimed that

PERTURBATION THEORY TERMINATES AT CORRECTION ORDER

$$Z^{-1/3}$$

I have spend a some time trying to prove this with no success.

Myron's Scholarship

Myron's scholarship was certainly much better than mine. His paper includes references that chart the history of the development of the Thomas-Fermi model.

In his Introduction, Myron notes: "That higher order terms are likely to be nonanalytic has been noted by Shakeshaft and Spruch [Phys. Rev. A **23**, 2118 (1981)]".

In the penultimate paragraph of his Introduction, Myron states that "We also note that any further corrections will be nonanalytic in $Z^{-1/3}$".

So my conjecture was 25 years behind the times.

At the end of Section III B, Myron asserts:

"If we attempt to calculate higher order terms, as, for example by the use of (3.3), and as neither μ nor $\tilde{\mu}$ will be zero the answers will have a ζ dependence and this will be nonanalytic in $Z^{-1/3}$."

This apparently is a proof of the conjecture.

But it is too terse for me to understand.

Poignant conclusion: I wish Myron were here to explain this to me.