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Fermi's favorite figure: the history of the pseudopotential concept in atomic physics and neutron physics

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Abstract In the early 1930's, Fermi wrote two papers in which he introduced the concepts of "scattering length" and "pseudopotential." Since that time, these terms have become universally associated with low energy scattering phenomena. Even though the two papers are very different—one in atomic physics, the other in neutron physics—a simple figure underlies both. The figure appears many times in Fermi's work. We review how the two papers came about and briefly discuss modern developments of the work that Fermi initiated with these two remarkable papers.

1 Introduction

Close to ninety years ago Fermi wrote papers defining two terms now universally used to describe scattering processes: "scattering length" and "pseudopotential." The papers discussed phenomena that could hardly be more different. The 1934 paper [9] focused on atomic spectroscopy, explaining the puzzling pressure shift of spectral lines in highly excited alkali metal atoms [1]. The 1936 paper [11] focused on the scattering of thermal neutrons from free protons and from protons bound in materials. But as Segre notes, p706, in his commentaries to Fermi's collected papers [13] "Fermi had a great insight for discerning analogies in phenomena which were completely unrelated."

Both papers do indeed have a common feature: a drawing, almost a sketch, of a radial wave function inside and outside a potential well. A version of the figure appears thirteen times in the collected works, six times in his nuclear physics notes [12] and became, as Segre notes further "... a sort of trademark in many of his (Fermi's) later theoretical studies."

In our paper here, we discuss the history of these two papers, the way the figure was utilized by Fermi, and how his thinking evolved between the first and the second publications. We think it is a useful exercise to go back and be reminded of the creative processes of one of the twentieth century's most innovative physicists. While both papers were first written in Italian, the second was subsequently translated into English [13] and is better known, to the extent that often the neutron paper is cited as the genesis of the idea of the pseudopotential. But primacy of the original ideas does lie with the first paper from atomic physics. The methodology he developed there for analyzing spectroscopic data continued to be cited into the 1980's [20]. And interestingly, most of the applications today of the pseudopotential concept lie in the field of atom–atom interactions in ultracold systems.

During this period, Fermi also wrote his primary papers [10] explaining beta decay. CN Yang relates [28] that Wigner considered this to be Fermi's most important contribution to physics. The figure does not appear there of course. But it does have a feature these other two papers have: squeezing what you do not know into an increasingly smaller volume—eventually a delta-function—and characterizing your lack of knowledge by a single number, G_F in beta decay, the scattering length a, for low energy scattering processes.

2 Fermi's paper of 1934

The goal of the paper was to explain shifts to higher energy of alkali metal absorption spectral lines due to the interaction with "foreign" neutral atoms. Of particular interest were transitions from very high lying levels, for

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example, 3S–30P in sodium. Simple Bohr model scaling puts the radius of the valence electron orbit at ~ 500 Å. At a gas pressure of one atmosphere, the electron can then collide with of order 13,000 foreign atoms in the atom volume. At this excitation energy, the valence electron is barely bound, with kinetic energy ~ 0.015 eV and de Broglie wavelength ~ 100 Å.

Atomic spectroscopy was a strength of Fermi's colleagues at Rome. In late 1933, Amaldi and Segre [1] had investigated pressure broadening of sodium spectral lines due to "perturber" atoms and had found puzzling results. They had expected the foreign gas to destroy the high terms of the absorption series, spreading the lines out so they were no longer clearly visible. That did not happen. Furthermore, they expected the spectral lines to always shift to the red. That did not happen either. In argon, the lines did shift red. But in nitrogen, they did not shift at all, and in hydrogen and helium, they shifted blue.

The shift to the red was based on the idea that the foreign gas atoms would be polarized by the residual field + e of the core of the alkali metal atom (Z protons, Z-1 electrons). This would lower the energy of the outer electron to account for the energy stored in the polarization electric field. A classical analogy would be a capacitor consisting of two spherical shells, with a dielectric consisting of foreign gas atoms in between the two shells. The energy is $U = \frac{1}{2}Q^2/C$ and with Q fixed as C increases by a factor k, the dielectric constant, the energy U of the system goes down.

Fermi introduced his own version of the polarization model. Taking advantage of a calculation by his colleague Wick [27], he confirmed that while the polarization shift had about the right magnitude, the effect was always to the red, lower in energy.[1] With the failure of the polarization model, Fermi then proceeded to look for an alternate explanation, this time focusing on the behavior of the valence electron as it travels slowly in its orbit.

Denoting R as the magnitude of the distance of the electron from the core of the alkali atom, and r as the magnitude of the distance of the electron from the perturbing neutral atom, he writes the Schrodinger equation for the wave function of the electron as:

$$\nabla^2\psi(r) + \left(\frac{8\pi^2 m}{h^2}\right)(\epsilon - U(R))\psi(r) - \left(\frac{8\pi^2 m}{h^2}\right)\sum_i V_i\psi(r) = 0 \tag{1}$$

Here, $V_i(r)$ is the potential well due to perturber atom i, and $U(R)$ is the weak and slowly varying coulomb attraction of the alkali atom core on the valence electron. The energy ϵ is the full energy of the alkali atom. In principle, $\boldsymbol{R}$ and $\boldsymbol{r}$ are vectors. But he is soon going to say U is essentially constant, and therefore, he can work with a one-dimensional Schrodinger equation in r alone.

To solve the equation with the unknown potential $V_i(r)$, Fermi takes advantage of the fact that for these very low energy electrons, only s-wave scattering is relevant. For the case of known potentials, the quantum theory of slow electrons scattering by atomic gasses (Ramsauer–Townsend effect) had already been studied in detail by Faxen and Holtsmark [8]. For the unknown potential, Fermi chooses to use a spherically symmetric potential of very short range ρ. He notes that because the atoms are neutral, the well is very narrow in relation to the de Broglie wavelength of the electrons.

He now introduces a new function, $\overline{\psi}$ that is a spatial average of the true wave function ψ over a distance that is large enough to contain many perturbers, but small enough so U (the weak Coulomb potential) can be considered constant. He argues that $\overline{\psi}$ reproduces the general trend of ψ but does not have the irregularities associated with the narrow but deep potential wells. Averaging yields a new equation:

$$\nabla^2\overline{\psi} + \left(\frac{8\pi^2 m}{h^2}\right)(\epsilon - U)\overline{\psi} - \left(\frac{8\pi^2 m}{h^2}\right)\sum_i \overline{V_i\psi} = 0 \tag{2}$$

To evaluate the third term, he notes that inside the well $V_i(r)$ is large and $(\epsilon - U)$ is negligible. For $r < \rho$, the Schrodinger equation therefore becomes, with $u(r) = r\psi(r)$,

$$u'' = \left(\frac{8\pi^2 m}{h^2}\right)V_i u \tag{3}$$

Far away from the origin ($r > \rho$), $V_i = 0$, $u'' = 0$ and the solution is simply $u = c_1 + c_2 r$. But far away, $\psi = \overline{\psi}$, $u = r\overline{\psi}$, and he can set $c_2 = \overline{\psi}$. At this point, the famous figure appears (Fig. 1). He introduces a new quantity a by writing $c_1 = a\overline{\psi}$. He does not give a name to a, but notes it is a "length" whose meaning is clarified by the figure. The perturber atom displaces the electron wave function by a distance a from the origin.

[1] In the appendix, we review his calculation in the light of extensive subsequent work by many to understand pressure broadening and shifting of spectral lines, a hugely important subject for astrophysics, atmospheric physics, and plasma physics.

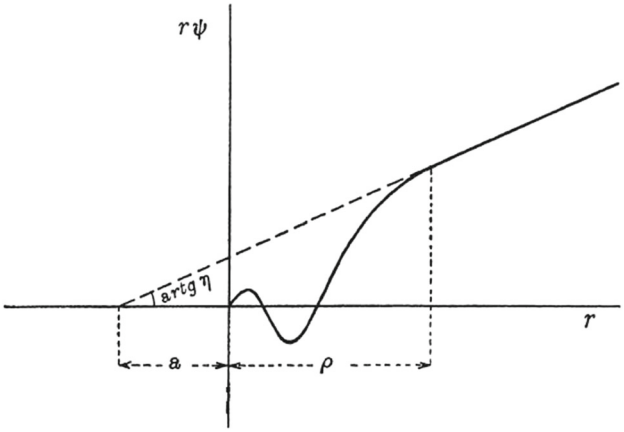

Fig. 1 Interpretation of the scattering length in [13], page 711

With the boundary condition $u(r=0)=0$, and the solution $u=(a+r)\overline{\psi}$ for large r, the third term in Eq. 1 can be evaluated by taking a volume integral:

$$\begin{aligned}\left(\frac{8\pi^2 m}{h^2}\right)\int V\psi \mathrm{d}\tau &= 4\pi\left(\frac{8\pi^2 m}{h^2}\right)\int Vur\mathrm{d}r \\ &= 4\pi\int u'' r\mathrm{d}r = 4\pi\left|u'r-u\right|_0^r = -4\pi a\overline{\psi}\end{aligned} \tag{4}$$

With n as the density of foreign gas "perturbers," Eq. 2 becomes a Schrodinger equation in the averaged wavefunction with an energy shift that is linear in the scattering length a, and in the gas density n:

$$\nabla^2\overline{\psi}+\left(\frac{8\pi^2 m}{h^2}\right)\left(\epsilon+\left(\frac{h^2 an}{2\pi m}\right)-U\right)\overline{\psi}=0 \tag{5}$$

The sign of a is not known so the shift could be in either direction. But the cross section for s-wave scattering from a potential well is well understood from the work of Faxen and Holtsmark. Amaldi and Segre find a cross section of about 12 Å^2, and from $\sigma=4\pi a^2$, they get a value for the scattering length of $\pm$ 1 Å.

With known values of a, n, m and Eq. (5), Fermi can explain the shifts of spectral lines in the Amaldi and Segre experiment. He publishes his results in March 1934.

The term linear in a in Eq. (5) is often called the Fermi "optical potential" and with the reduced Plank constant is written as

$$V=\frac{2\pi\hbar^2}{m}an. \tag{6}$$

Many contemporary authors also call it the Fermi "effective" potential, having in view that it leads, approximately, to the same results as the true potential. But at this point, Fermi is not using this terminology. For him, the potential well due to the perturber atom is simply deep and narrow. It becomes a delta function only in the 1936 paper, which we now discuss.

3 Fermi's paper of 1936

In the collected works [13], p 639, Segre notes that up to 1934, Fermi's work had been mainly theoretical. But with the discovery of the neutron in 1932, and the feeling among his experimental colleagues that atomic spectroscopy had run its course, focus shifted toward nuclear physics, and particularly to experimental neutron physics. Segre further notes: "The occasion for a really new departure in the nuclear field occurred in 1934 with the discovery by I. Curie and F. Joliot of artificial radioactivity." Fermi's group had access to a gram of radium and could generate neutron beams by alpha bombardment of beryllium. There followed an intense period of experimental activity, much in collaboration with Amaldi who notes in [13] p 808: "We had prepared a systematic plan of attack which

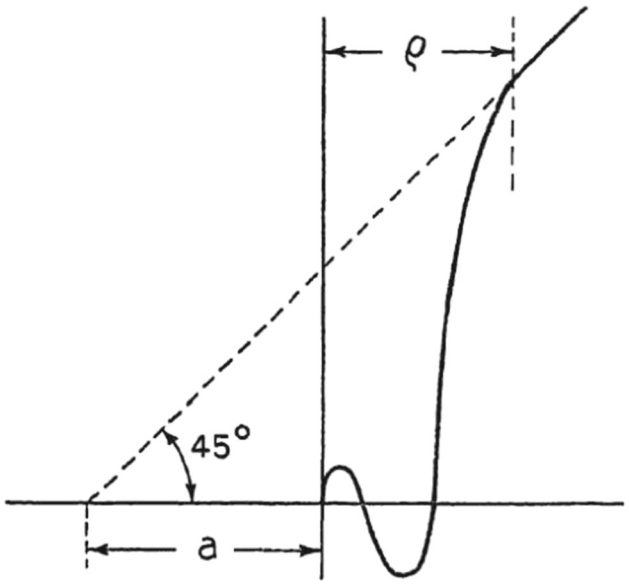

Fig. 2 Interpretation of the scattering length in [13], p 969

we jokingly summarized by saying that we would measure the absorption coefficient of all 92 elements combined in all possible ways with 92 elements used as detectors."

The 1936 paper is, however, a theoretical paper, first published in Italian. Amaldi comments: "In addition to many new results, it contains some results obtained earlier, but previously unpublished, or published only in preliminary form." Amaldi tried to convince Fermi to translate the paper into English. But apparently, Fermi replied along the lines: "I don't want to waste the time, and if someone was interested in studying slow neutrons, he would have to read it, even if it was published only in Italian." It was of course later translated by Temmer. Both the Italian original and the English translation appear in [13], one of only a handful of papers to get "star treatment".

Fermi proceeded in the same way as in his 1934 paper, however, without any reference to it. The goal was to introduce an average potential for interaction of a neutron at coordinates (x,y,z) with a proton at coordinates (X,Y,Z). The proton is chemically bound in a hydrogenous medium. Various length scales are introduced. The nuclear potential range, ρ, is of order 10^{-12} cm. The chemical bonding potential is denoted $U(X,Y,Z)$ and acts over a scale of the order of the amplitude of atomic vibrations in a molecule, about 10^{-9} cm. Slow neutrons have wavelengths λ of order 10^{-8} cm. The true wave function is $\psi(x,y,z,X,Y,Z)$.

Proceeding as in 1934, he introduces a wave function $\overline{\psi}$ that is averaged over a sphere of radius R. He gives more detail about what calculating the average means than in the previous paper, but basically the result is the same. The radius R satisfies the inequalities:

$$R \gg \rho \quad \text{and} \quad R \gg a, \quad \text{but}\, R \ll \lambda. \tag{7}$$

The scattering length a appears again, but in a new version (Fig. 2). The averaged wave function is now normalized to unity so $u = r\psi = (a + r)$ and the angle is 45 deg.

Finally, Fermi obtained the desired Schrodinger equation for $\overline{\psi}$, this time in its time-dependent form:

$$-\frac{h}{2\pi i}\frac{\partial\overline{\psi}}{\partial t} = -\left(\frac{h^2}{8\pi^2 M}\right)\left\{\frac{\partial^2\overline{\psi}}{\partial x^2} + .. + \frac{\partial^2\overline{\psi}}{\partial X^2} + ..\right\} + U\overline{\psi} - \left(\frac{h^2 a}{\pi M}\right)\delta_R(r) \tag{8}$$

The new function $\delta_R(r)$ he defines to be equal to $3/(4\pi R^3)$ for $r < R$ and to be zero for $r > R$. Its volume integral extended over all space is equal to 1. And since the quantities in Eq. (8) vary slowly in the region where $\delta_R(r) \neq 0$, Fermi wrote that, in the first-Born approximation, "... when calculating the matrix elements of the interaction term, the function $\delta_R(r)$ may be identified with the Dirac delta-function in three dimensions."

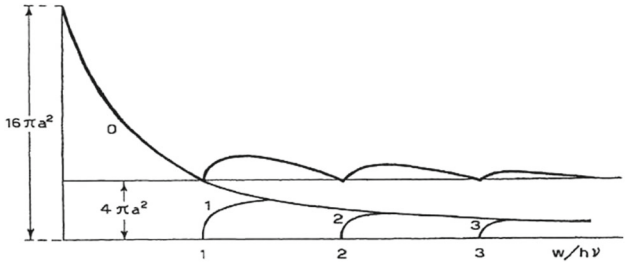

Fig. 3 Neutron elastic and inelastic cross sections in paraffin [13], p 973

This is the essence of the Fermi pseudopotential concept. In modern notation [24], it is written[2]:

$$V_{\boldsymbol{F}} = 2\pi\frac{\hbar^2}{m}nb\delta^{(3)}(r). \tag{9}$$

Here, $b = \left(\frac{A+1}{A}\right)a$ is the bound scattering length for a nucleus of mass number A, and n is the number density of scatterers.

Fermi applied the first-Born approximation to tackling the problem of inelastic scattering of neutron in paraffin while treating the hydrogen atoms as harmonic oscillators of frequency ν. He calculated, for the first time, the elastic and inelastic cross sections in the function of the neutron energy w, which are shown in Fig. 3. The curves 1, 2, 3 correspond to excitations of the oscillator in the corresponding excited states. This theoretical prediction was confirmed experimentally only about fifteen years later.

We've been writing the term scattering length here, but it is somewhat unclear when Fermi started using it. The first appearance in a publication is in 1947 in Fermi and Marshall [15]. He was, however, using the term in 1945 in (at the time) classified lectures. The neutron scattering sections were later declassified and are reproduced from participant notes in volume two of the collected works [14] p469.

Interestingly, the definition of the sign of a changed during this time. Earlier he had taken a to be positive when the intercept fell to the left of the origin because this made the (unbound) singlet n–p scattering length positive. But as more data were accumulated, it became clear that hydrogen was an unusual case, and most scattering lengths were of the opposite sign. By the time of the Fermi and Marshall paper in 1947, he adopts the modern (negative) sign convention for the relation between the phase shift δ and the scattering length a as the wavenumber k goes to zero: $\delta = -ka$.

As more and more data were accumulated, the accuracy of what became known as "Fermi method"—Fermi potential plus first-order Born approximation—became a focus of theoretical work by others. Breit [4] noted that the original version of the pseudopotential defined over a sphere of radius R with the factor $\delta_R(r)$ was problematic because it implied an interaction energy inside the potential well of $V = \frac{3a}{R}\frac{h^2}{MR^2}$. This gives a scaling law VR^3, not the expected VR^2. But he found that when used in scattering problems to first-order Born approximation, the delta function version of the potential was very reliable. For free protons, Breit reproduced all Fermi's results and for bound protons, found the corrections were only of order 0.3%. The conclusion was that the application of the first-order Born approximation with the Fermi pseudopotential does not increase the typical inaccuracy of the Born method. Later, Blatt and Weisskopf [2] came to the same conclusion.

4 Modern applications of the scattering length and pseudopotential concepts

In Fermi's original thinking about a low energy scattering process, the fine details of the unknown short-range interaction potential were not relevant, and the situation could be described completely by one parameter, the scattering length, or equivalently the pseudopotential. This idea has continued to bear fruit with remarkable consequences in systems as varied as Bose–Einstein condensates, where the scattering length can be adjusted to any value by external magnetic fields—Feshbach resonances—to few body stems where quantum mechanics predicts the formation of bound trimers—Efimov states—many times bigger than the range of the interaction itself.

Resonances in neutron reactions are a common phenomenon, arising when the energy of the incoming neutron matches the energy of a discrete state in the compound system. Feshbach, thinking primarily about nuclear

[2] See [24] for clarification on the terminology and distinctions between the potentials in Eqs. (6) and (9).

reactions, showed [16] that this was a general feature of any collision process. Feshbach resonances in atomic physics came into play because the magnetic interactions in atoms are dependent on the magnetic moments of nuclei through the hyperfine splitting of the energy levels of the total angular momentum. Theorists developed two channel zero-range potential models, calculated the scattering length, and found resonance behavior in the dependence of the external magnetic field.

Inoue et al. [18] confirmed these predictions by manipulating the scattering length in a ^{23}Na Bose–Einstein condensate exposed to a spatially homogeneous magnetic field of variable strength. For a review, see Chin et al. [5]. The phenomenon is named after Feshbach who, as related by Kleppner [19], found it amusing that his name should be attached to such a generic phenomenon. Today, the method is widely used to tune the interactions between ultracold atoms over many orders of magnitude in atomic Bose and two-spin-component Fermi gasses. An abstract search in arxiv.org lists over 1600 references to the term "Feshbach resonance."

Feshbach's technique developed for nuclear processes found its most fruitful applications in atomic physics. Similarly, calculations [6] aimed at understanding the structure of three body nuclear systems—the triton, the Hoyle state in 12C—subsequently found remarkable confirmation in three body atomic systems. Efimov considered a system in which three particles are interacting pairwise through short-range potentials that are not quite strong enough to bind but are nearly in resonance, so the respective scattering length is large. The singlet n–p scattering length is an example: $a = 23.5$ fm compared to a typical nuclear force range of a few fm. He found that when three identical bosons are present, a bound-state system emerges with size comparable to the scattering length, not the nuclear force range. Counterintuitively, he found a whole series of bound states $n = 1, 2, 3\ldots$, with sizes increasing by factors of $(22.7)^n$ each time, and bound-state energies scaling as $1/(22.7)^{2n}$. This strange numerical factor ($e^{\pi/|s_0|}$, with $|s_0| \approx 1.00624$) emerges from zero-range theory, and this power law scaling is coming from the fact that the overall potential has a $1/r^2$ behavior, well known for its paradoxical properties.

It took 35 years to confirm Efimov's predictions, in part because you need to identify both a ground and an excited state to confirm the size and energy scaling predictions. See Naidon and Endo [22] and Braaten and Hammer [3] for a full discussion and complete references. Efimov recounts the history of his prediction in "Giant trimers true to scale" [7] and notes "it has been heartening to witness the evolution of this miracle of quantum mechanics from questionable to pathological to exotic to being a hot topic of today's ultracold physics." Perhaps as nuclear physics explores the edges of the valley of stability with new radioactive ion facilities like FRIB, we may hope to identify more barely bound systems that link back to Efimov's original predictions and their roots in the world of nuclear structure.

5 Conclusion

From the outlined history of the Fermi pseudopotential concept one can conclude the following:

- The so-called *effective* or *averaged* potential, V, (Eq. 6) in the Schrodinger equation for interaction of electrons with the media was first introduced by Fermi in 1934. About twenty years later, in neutron optics, it got the name optical potential.
- The *pseudopotential* with the *Dirac Delta*-function, V_F, (Eq. 9) allowing calculations in the first Born approximation, appeared in the neutron physics paper published in 1936. Under the notation V_F it is known since Breit's paper of the year 1947.
- The most active use and development of the Fermi pseudopotential concept are presently in the field of ultracold atom physics where Efimov states and Feshbach resonances are yielding fascinating new insights into the quantum world. New radioactive beam facilities like FRIB may provide more surprises as they explore nuclear structure far from the line of stability.

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Appendix A: History and later developments in understanding pressure broadening of spectral lines

In the main text, we discussed the history of the Fermi pseudopotential and how the term came to be universally adopted. We noted that his analysis of the Amaldi–Segre Rydberg atom data involved breaking the line shift due to perturber atoms into two parts: one (larger) due to electron-perturber atom scattering, the other (smaller) due to polarization of the perturber by the Rydberg atom core. Our focus was on the electron-atom scattering that lead to the concept of the scattering length. But it is interesting to note that his calculation of the smaller core polarization contribution was also the starting point of many decades of work by others to understand spectral line shifts and pressure broadening in ever more detail.

Fermi's calculation of the core polarization contribution followed from writing down the polarization energy ΔE of a perturber atom due to the electric field e/R^2 of the alkali atom core. With α as the atomic polarizability, this change in energy is $\Delta \mathrm{E} = \frac{1}{2}\alpha e^2/R^4$, where R is the distance from the core to the perturber. This will be infinite if R can go to zero, but, working with Wick [9] and possibly being aware of extensive work by Holtsmark [17] they realize that the most probable distribution of 1500 or so perturbers is a uniform distribution in space. At this point, Wick proceeds to calculate the probability distribution $P(\sigma)$ of $\sigma = \sum_{i=1}^{\infty} 1/x_i^{4/3}$ where $x_i = \left(\frac{4\pi}{3}\right)R_i^3 n$ and n is the number density of perturbers. He finds that the probability distribution has a broad spread but peaks at $\sigma = 2.8$. He submits his results for publication in December 1933 [27]. Fermi takes a possibly earlier value from Wick, however, and initially uses 2.6 in his paper. But he then rounds it up to an overall factor of 20 since he knows from Wick that the distribution of probability values is asymmetric. Fermi's final result for the shift (published March 1934) is

$$\Delta \mathrm{E} = -\frac{1}{2}\alpha e^2 n^{4/3} \times 20$$

Barely more than a year later, both the scattering length plot and the polarization calculation have been picked up by Margenau and Watson (MW) in a January 1936 paper [21] on pressure effects in spectra lines. In that paper, they gave a two-line derivation of the Wick result, and from this time on this simple derivation is referred to as "the Fermi method."

The MW calculation assumes the perturbers are uniformly distributed in volume, and that the shift is dominated by the nearest perturber at radius R_1 given by $\left(\frac{4\pi}{3}\right)R_1^3 n = 1$. Accordingly, they write $\sum_{i=1}^{\infty} 1/R_i^4 = \int_{R_1}^{\infty} 4\pi n R^2 \mathrm{d}R/R^4 = 4\pi n/R_1 \approx 20\, n^{4/3}$ which gives essentially the same factor Fermi came up with. The closeness of the MW result to the value Fermi finally used in his 1936 paper leads one to speculate that Fermi with his unmatched physical intuition might have had this simple calculation in mind. But he did not actually publish it so credit should go to MW, even though MW do call it "Fermi's theory."

The radius R_1 is called the Wigner–Seitz radius. Earlier, noting that the perturber could also feel the influence of the core at a distance that depended on how fast the perturber atom was moving [26], Weisskopf had introduced the concept of the Weisskopf radius. A more complicated picture emerged as it was realized [25] (and confirmed experimentally [20]) that line broadening was primarily due to perturbers inside so-called Weisskopf sphere, while the line shift was primarily due to perturbers outside the Weisskopf sphere. Today the theories are much advanced, with classical trajectories replaced by full quantum mechanical calculations based on formal scattering theory [23].

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