

# On History of the Fermi Pseudopotential Concept in Atomic and Neutron Physics

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## 1. Introduction

This report will bear a touch of history. Enrico Fermi introduced the pseudopotential concept about 85 years ago. The Collected Papers of Fermi [1, 2], published in 1962 by the University of Chicago Press, revealed that this happened in 1933–1934. Fermi group just finished their studies in atomic spectroscopy, published their results and switched to a search of radioactivity induced by neutrons. Besides Fermi the Photo of [3] shows also physicists Franco Rasetti, Eduardo Amaldi, Emilio Segre and chemist Oscar D’Agostino.



Photo of [3]: Fermi group in 1934.

On January 27, 1934 Amaldi and Segre published the paper [4] on the shifts of high terms of alkaline atomic spectra in the presence of an additional (“foreign”) gases H, He, Ar, O<sub>2</sub>, and N<sub>2</sub>. After active discussions with Amaldi and Segre, Fermi had found the explanation of the effect. In the end of 1933 he sent the paper [5] to *Nuovo Cimento*. The following quotation is from comments of Emilio Segre to paper [5] in [1]: “*We meet there for the first time the concept of the scattering length and of ‘pseudopotential’. This theoretical development is remarkable... it gives a technique that Fermi used many times in connection with his neutron works*”. However, according to numerous reviews and books in neutron physics, Fermi introduced the pseudopotential for the first time in his seminal paper [6] in

1936 on physics of thermal neutrons behavior in paraffin and water. There is an unsettled issue here. Therefore, I'll give some details of both papers first, and then will proceed to rather general examples of how Fermi pseudopotential became a powerful concept for the latest developments in several research fields, such as ultracold neutrons, ultracold atoms, and condensed matter.

## 2. Fermi's paper of 1934

The most essential goal of paper [5] was to explain the shift of the spectral lines due to the interaction of the alkali atom valence electron with 'foreign' neutral atoms. Fermi estimated that due to a rather large radius of such electron orbit and the gas pressure of  $\approx 1$  atm, there should be about  $10^3$  of foreign atoms in the alkali atom volume where the electron can collide through the potentials  $V_i(r)$ . Using the Schrodinger equation in its historic form of 1926:

$$\Delta\psi(r) + \gamma(E - V(r))\psi(r) = 0, \quad \text{with: } \gamma \equiv 8\pi^2m/h^2, \quad \Delta \equiv \nabla^2,$$

Fermi, for his problem, wrote

$$\Delta\psi(r) + \gamma(W - U - \sum V_i(r))\psi(r) = 0. \quad (1)$$

The energy  $W$  here is the full energy  $E$  for the alkali atom,  $U$  is a weak remnant of the closed shell potential and  $r$  is the electron distance relative to neutral atom. As an example, the Lennard-Jones potential for interaction of two neutral molecules is shown in Fig.1. Its effective range value is  $\rho \approx 6 \text{ \AA}$  and its known analytical form allows exact solutions of practical problems.

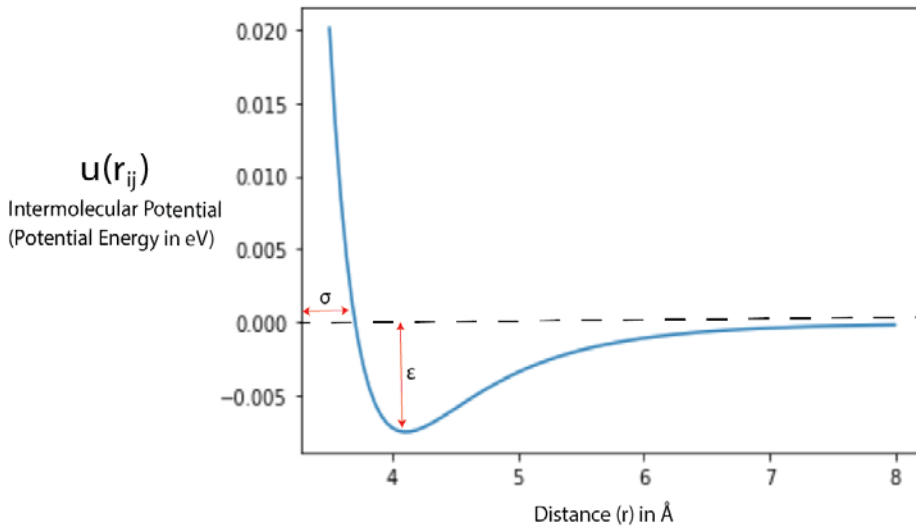


Fig.1. The Lennard-Jones potential.

To solve the Schrodinger equation with unknown potential  $V_i(r)$ , Fermi formulated an approximation presently known as one of simple forms of the boundary condition method. He considered a spherically symmetric (s-wave scattering) potential  $V_i(r)$  and introduced, in addition to the exact wave function  $\psi(r < \rho)$ , the function  $\Psi$  by averaging  $\psi$  over the distances  $r$  in a broad region included the potential "well"  $V_i(r)$  (at  $r < \rho$ ) and the space outside (where  $V_i(r) = 0$ ). This region was taken to be less than the de Broglie wavelength for the electron ( $\lambda_B$

$\approx 100 \text{ \AA}$  here), but large enough to contain many foreign atoms. The function  $\Psi$ , as opposite to  $\psi$ , has no singularities through all the considered space. Using the relationship  $\Delta\Psi = \langle \Delta\psi \rangle$  for averaging Eq. (1), Fermi wrote the Schroedinger equation for the averaged function in the form:

$$\Delta \Psi(r) + \gamma(W - U)\Psi - \gamma \langle \sum_i V_i(r)\psi(r) \rangle = 0. \quad (2)$$

To calculate the value of the last term in this equation he introduced another function,  $u(r)$ , by the replacement  $\psi = u(r)/r$ , usually used for the case when  $V_i(r) = 0$ , and applied it for all  $r$ . The reasons for the replacement was the linear behavior  $u(r) \sim (a + r)$  for this function outside the potential “well” and the obvious boundary condition  $u(r=0) = 0$ .

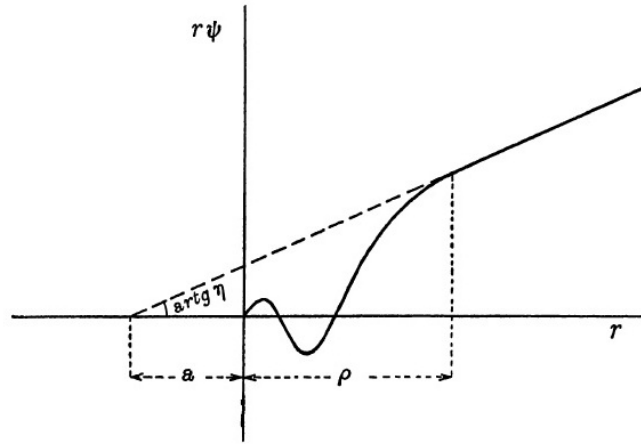


Fig.2. Interpretation of the scattering length  $a$  in [5].

The constant  $a$  was already used in the theory of atomic collisions as the limit of the ratio  $a = \delta(k)/k$  at  $k \rightarrow 0$ , with  $\delta(k)$  the phase shift of the scattered wave and  $k$  is the wave number. By plotting the function  $u(r) = r\psi$ , Fermi introduced another interpretation of  $a$  as the ‘scattering length’. This famous plot is shown in Fig. 2.

Using Eq.(2) without the small term  $U$ , Fermi deduced the differential equation for  $u(r)$  at ( $r < \rho$ )

$$u''(r) = \gamma V(r)u(r). \quad (3)$$

All these relationships were used to calculate the contribution of an one  $i$ -term (one ‘well’) in the sum, Eq.(3), by taking the volume integral

$$\gamma \int V\psi d\tau = 4\pi\gamma \int Vudr = 4\pi |u''r - u|_0^r = -4\pi a \Psi. \quad (4)$$

Introducing  $n$  as the number of foreign gas ‘potential wells’ per  $\text{cm}^3$ , Fermi finally obtained the equation

$$\Delta \Psi + \gamma(W - U - \frac{\hbar^2 a n}{2\pi m})\Psi = 0. \quad (5)$$

The third term in Eq.(5) is *presently* often called the ‘optical potential’ and written as

$$V = \frac{2\pi\hbar^2}{m} an. \quad (6)$$

With known values of  $a$ ,  $n$ ,  $m$  and Eq.(5) Fermi had explained the shifts of spectral lines in the Amaldi and Segre experiment.

### 3. Fermi's paper of 1936

The 1936 paper [6] was also published in the Italian translated into the English later in [1]. The paper is well known, referenced in all books, therefore the details will be omitted, and only the salient points, which distinguish it from the paper of 1934 will be given here. The goal was to introduce an average potential for interaction of neutrons with protons chemically bound in a hydrogen medium. While the scale of the nuclear potential range is of the order of,  $10^{-12}$  cm, the regions where the chemical bounding forces work is of the order of amplitudes of atoms vibrations in the molecule, that is, about  $10^{-9}$  cm. Using now  $U(X,Y,Z)$  as the potential energy of chemical forces, introducing again, in addition to the full true wavefunction  $\psi$ , the new function  $\Psi$  by performing an appropriate averaging this time over a large sphere of radius  $R$  around the neutron position, assuming that the length  $R$  simultaneously satisfies the inequalities

$$R \ll \lambda; \quad R \gg \rho; \quad R \gg a, \quad (7)$$

Fermi proceeded further in exactly the same way as in 1934 paper [5], however without any reference to it, and had shown the drawing, Fig. 3, analogous to Fig. 2:

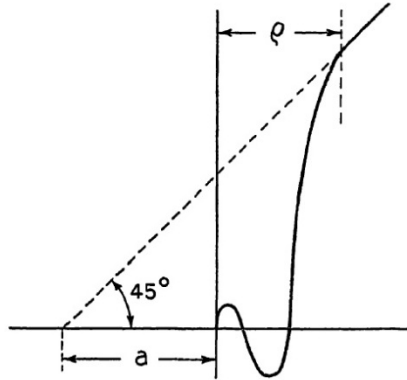


Fig.3. Interpretation of the scattering length  $a$  in [6].

Finally, Fermi obtained the desired equation for  $\Psi$ , which we show in a slightly different form than given in [6]:

$$\Delta \Psi + \gamma(W - U - (\hbar^2 a / \pi M) \delta_R(r)) \Psi = 0. \quad (8)$$

The new function  $\delta_R(r)$  he defined to be the equal to  $3/(4\pi R^3)$  everywhere 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 the statement that, in the first Born approximation, we quote, "... when calculating the matrix elements of the interaction term in Eq.(8), the function  $\delta_R(r)$  may be identified with the Dirac delta-function in three dimensions". This is the essence of the Fermi pseudopotential concept. The pseudopotential itself, in the modern notation, is

$$V_F = 2\pi \frac{\hbar^2}{m} a \delta^{(3)}(r). \quad (9)$$

Fermi applied the first Born approximation with this potential for tackling the problem of inelastic scattering of neutron in paraffin while treating the hydrogen atoms as harmonic oscillators of frequency  $\nu$ . 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.4. 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.

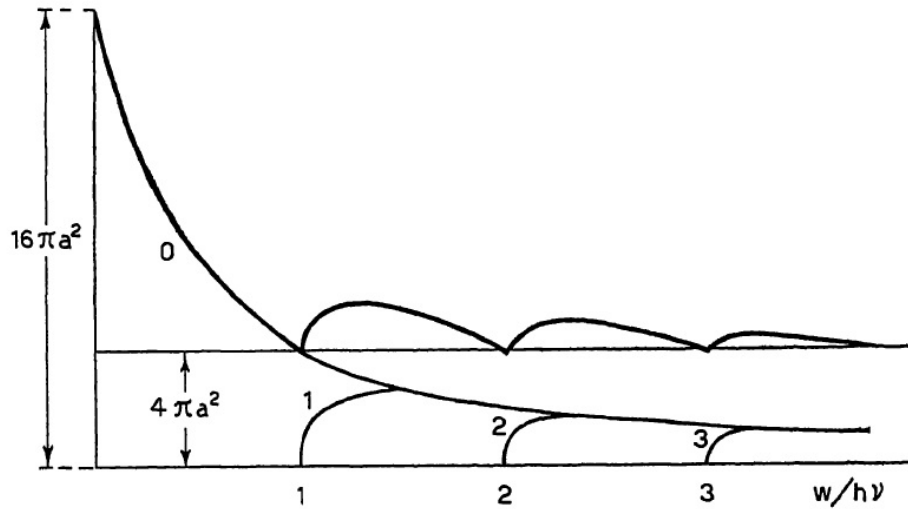


Fig.4. Neutron elastic and inelastic cross sections in paraffin.

#### 4. Further developments in neutron and atomic physics

**The neutron physics field.** Ten years later, Gregory Breit [7], considering the Fermi method as the first approximation to the possible more accurate equations, formulated the same problem in terms of the boundary conditions method with the integral equations. The paper [7] is entitled:

*G. BREIT*

*The scattering of slow neutrons by bound proton.*

To describe nuclear properties within the exact approach, Breit applied the ‘intercept’ quantity  $a$ , which he named the *Fermi scattering length*. For the free protons case, the Fermi result was obtained again. For the bound protons, Breit calculated the correction of only 0.3%. The final resume was that the application of the first Born approximation with the Fermi pseudopotential doesn’t increase the typical inaccuracy of the Born method. Later J.M. Blatt and V.F. Weisskopf [8] in their *Theoretical Nuclear Physics* came to the same conclusion.

The next fruitful phase in developing of the theory was focused mainly on properties of the many body wave functions of scattering, in particular on multiscattering corrections to the optical potential. This is a separate topic for recollections and reviews, requiring a special mathematical background. For an introduction to it one may start with the paper [9]:

*A.L.BARABANOV, S.T. BELYAEV*

*Multiple scattering theory of slow neutrons (from thermal to ultracold).*

The recent papers of Yu. Pokotilovski [13] and H. Abele [14] review the present status of the experimental researches with ultracold neutrons. In this field, the so-called ‘optical potential’, based on the Fermi method, is widely used and serves nowadays in precision studies of neutron beta-decay for the Standard Model tests and for searches of a ‘new physics’.

**Atomic physics field.** After the invention of the laser sources of the coherent light (with the Nobel Prize awarded in 1964), the atomic physics experienced a second birth, especially when techniques of cooling and trapping atoms with laser light and magnetic fields (the Nobel Prize awarded in 1997) became widely available at universities of the USA, Europe and Asia. The explosion of research in atomic and molecular physics, that followed the new technology, was culminated by the experimental demonstration of the phenomenon of Bose-Einstein condensation in dilute gases of ultracold alkali atoms (with the Nobel Prize awarded in 2001). Essential for this progress were new approaches to modeling and new methods to calculate the atom-atom interactions in environments, such as magnetic and optical traps. As an introduction to the achieved results in this prolific field, one may see the paper [10] by S. Inouye et al., entitled “Observation of Feshbach resonances in a Bose-Einstein condensate”, the paper [11] by N.T Zinner, entitled “Effective potential for ultracold atoms at the zero crossing of a Feshbach resonance”, or the review [12] by Cheng Chin et al., entitled “Feshbach resonances in ultracold gases”. In atomic physics, the Schroedinger equation  $\mathbf{H} \Psi = E \Psi$  for the relative motion of two cold atoms contains, generally, a more complicated operator  $\mathbf{H}$ :

$$\mathbf{H} = -\frac{\hbar^2}{2m} \Delta + \sum \frac{\omega^2}{2m} r^2 + \mu B(r_i) + 2\pi \frac{\hbar^2}{m} a \delta^{(3)}(\mathbf{r}) \frac{\partial}{\partial r} r. \quad (10)$$

The second term here is the harmonic oscillator potential of the interacting atoms at the positions  $r_i$  in a trap, the third term is the interaction with the magnetic field  $B$  and the last term is the so-called *regularized* zero-range potential. It is required for the mathematical correctness when using the  $\delta^{(3)}$  function in three dimensions.

The phenomenon of the Feshbach resonances in nuclear physics is due to the coupling of the two channels in the collision: discrete nuclear state and the continuum region of the potential. The Feshbach resonances in atomic physics came into the 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 atom total angular momentum. Theorists developed the coupled two channel zero-range potential, calculated the scattering length  $a$ , and found the resonance behavior in dependence of the external magnetic field.

The result of the experiment for sodium atoms, shown in Fig.5 [10], demonstrates such behavior: at the resonance position  $B_0$ , the scattering length diverges ( $a \rightarrow \pm \infty$ ). Near the resonance, the function  $a(B)$  can be described as  $a(B) = a_{bg}(1 - \Delta/(B-B_0))$ . The physical output from this phenomenon is the association of interacting cold atoms into the cold molecules with a corresponding decrease of the initial atomic density (the upper part of Fig. 5).

This phenomenon was confirmed experimentally in several cases and opened the way to study the Bose-Einstein condensation in gases by tuning effective atomic interactions.

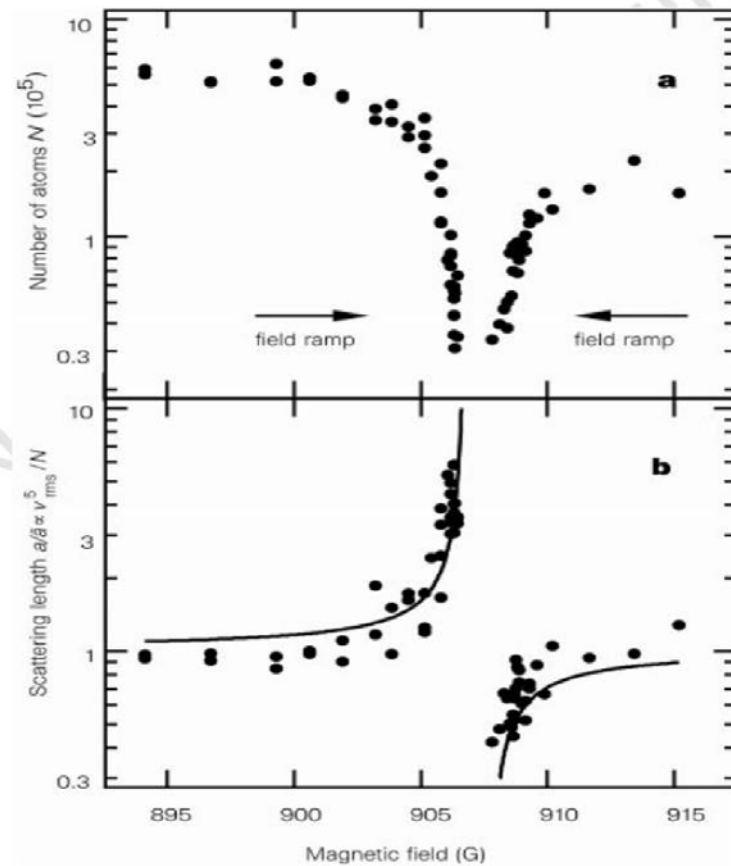


Fig.5. Feshbach resonance in Na.

### Conclusion

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

- The so-called effective or averaged potential,  $\mathbf{V}$ , in the Schroedinger 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,  $\mathbf{V}_F$ , allowing calculations in the first Born approximation, appeared in the neutron physics paper published in 1936. Under the notation  $\mathbf{V}_F$  it is known since the G. Breit's paper of the year 1947.
- To use the effective potential  $\mathbf{V}$  under the name "the *Fermi optical* potential" is not correct in a strict sense. History definitely made the choice of the Fermi name for "the Fermi pseudopotential"  $\mathbf{V}_F$ , in another words – "the Fermi zero-range potential".
- The most active use and development of the Fermi pseudopotential concept is going on presently in the field of the ultracold atoms physics.

### 5. Acknowledgment

Finally, many thanks are to Alexander Vladimirovich Strelkov. He often drew my attention to the physics beyond neutrons and, in particular, through his paper in [15], initiated this report and helped to work on it.

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