Russian Journal of Mathematical Physics, Vol. 12, No. 2, 2005, pp. 151–160.

On the Theory of Multiple Scattering of Waves (MSW) and the Optical Potential for a System of Point-Like Scatterers. An Application to the Theory of Ultracold Neutrons

J. Brüning*, S. Yu. Dobrokhotov, V. A. Geyler***, and T. Ya. Tudorovskiy****

**Institut für Mathematik, Humboldt Universität zu Berlin,*
Rudower Chaussee 25, 12489 Berlin, Germany
E-mail: bruening@mathematik.hu-berlin.de
***Institute for Problems in Mechanics*
(Russian Academy of Sciences)
E-mail: belov@amath.msk.ru, dobr@ipmnet.ru
**** ???????????*

Received March 30, 2005

Abstract. Nowadays, one of the main problems in the theory of ultracold neutrons (UCN) is that the actual time of their storage in closed vessels (the so-called "Zeldovich bottles") is by more than an order of magnitude smaller than the time predicted in the theory [1–3]. We model the neutron–nuclei interaction by using the point potentials and thus analyze the process of passing to the so-called "optical potential" [2, 4, 5] and the corrections arising as the result of this passage. We show that, in the case of many scatterers, the difference between the reciprocal scattering length a^{-1} at the jth scatterer and the same value at an isolated nucleus can be $\sim R^{-1}$, where R is the minimal distance between the scatterers. The optical potential is derived with the same accuracy. For the case in which the correction is assumed to be a random variable, the omitted terms can apparently be taken into account by adding an imaginary correction $\sim R^{-1}$ to the reciprocal scattering length in the optical potential. We consider a model in which the reciprocal scattering length is assumed to be a Lorentz distributed random variable. Using the so-called "supersymmetric trick" [6, 7], we explicitly obtain the averaged optical potential (the Fermi pseudopotential). The averaged optical potential turns out to be dissipative, and the imaginary correction to it coincides with the Lorentz parameter of the distribution.

1. INTRODUCTION

In 1959, Zeldovich [8] theoretically predicted that very slow neutrons can be stored in material traps, the so-called "Zeldovich bottles." It was shown that the interaction between slow neutrons and an ensemble of identical fixed point-like scatterers can be described by introducing the effective "optical potential"[1]

$$V = 2\pi\hbar^2 na/m, \tag{1}$$

where $\hbar$ is the Planck constant, n is the number of scatterers per unit volume, a is the so-called "scattering length" (a characteristic of the scatterer), and m is the neutron mass. This description is valid if the neutron wavelength is much greater than the distance $n^{-1/3}$ between neighboring scatterers. For the majority of matters, we have $a > 0$ and hence the optical potential is a positive potential of height $\sim 100\,\mathrm{neV}$, i.e., it is an effective potential barrier for incident particles. The incident neutrons with energies less than the barrier height are completely reflected. The neutrons with energies $\sim V$ were called *ultracold neutrons* (UCN).

The optical potential simplifies significantly the initial scattering problem for the the very slow neutron which interacts with the ensemble of fixed nuclei. The initial statement of the problem is the following.

One considers the stationary scattering problem for the slow particle, which interacts with the ensemble of the N fixed nuclei. We assume that jth nucleus with the centrum in the point $\mathbf{R}_j$

[1]The idea of the "optical potential" was appeared earlier in the rather different physical situation (see e.g. [9]).

is described by the potential U_j. For simplicity we assume U_j to be spherically symmetric, i.e. $U_j = U_j(\mathbf{r} - \mathbf{R}_j)$. The scattering state $\psi(\mathbf{r}, \mathbf{k})$ is the solution of the stationary Schrödinger equation with Hamiltonian H:

$$H\psi = E\psi, \qquad H = -\frac{\hbar^2}{2m}\Delta + \sum_{j=1}^{N} U_j(|\mathbf{r} - \mathbf{R}_j|) \tag{2}$$

with the radiation condition on the infinity of the form $\psi|_{r\to\infty} \to e^{i\mathbf{kr}} + f(\mathbf{kr})e^{ikr}/r$. There are two explicit parameters in this problem, namely kr_0 and kR, where r_0 is the characteristic radius of the nucleus and R is the characteristic distance between the nuclei. We want to construct asymptotic solution of the problem when $kr_0 \ll kR \ll 1$ ("ultracold" limit). It was shown in [2, 4, 5] that in this limit to calculate the asymptotic behavior of the wavefunction $\psi(\mathbf{r}, \mathbf{k})$ when $r \to \infty$ one can replace nuclei, i.e. $\sum_{j=1}^{N} U_j$ in (2), by the optical potential V given by (1).

So far the elastic and nonelastic interaction of UCN with matter has intensively been studied both experimentally and theoretically. The keen interest in this problem is motivated by the fact that the time of storage of neutrons in traps is much less than its theoretical estimates [1–3, 11].

Significant losses of neutrons in traps are caused by numerous collisions of neutrons with the trap walls, and in this case the coefficient of losses "per an impact" is a sufficiently small quantity. Phenomenologically, the losses can be taken into account by introducing an imaginary correction to the potential $V \to V' + iV''$, but the problem of justifying such a correction is still open. In [3, 5, 12, 13], it is assumed that the optical potential always contains a small imaginary correction, while in [2] it is stated that the optical potential is real if there is no absorption of neutrons by nuclei. These statements concern the case of fixed nuclei. Physically, the existence or absence of "imaginary terms" in the optical potential may depend on whether all the processes (channels) or some of them describe the optical potential.

We want to check two questions: 1) what is the accuracy of the derivation of the optical potential and 2) whether the optical potential concludes small imaginary part. These two questions are closely connected. Actually, if the accuracy of the derivation is insufficient, we can always include small imaginary part in the potential. Thus to answer this question one has to obtain, in principle, all terms of the expansion with respect to k. But the problem (2) is extremely complicated. So, at first, we are going to replace it by the *explicitly solvable* model, which is a good approximation of (2) when $k \to 0$. We show later that to this end one can consider the problem with point potentials as the model problem satisfying above conditions.

In the present paper, we consider apparently a new aspect of the problem of interaction between the neutron and an ensemble of identical fixed scatterers. Namely, we first show that even for identical scatterers, the scattering length cannot be assumed to be constant. The reciprocal of the scattering length is determined up to the order of the inverse distance between the neighboring scatterers. The fact that the crystal is nonideal and there are boundaries, heat motion of nuclei, impurities, etc. allows one to assume that this correction is a random variable. We show that, for the Lorentz distributed scattering lengths, the usual derivation procedure allows one to obtain the optical potential containing an imaginary correction depending on the parameter of the Lorentz distribution.

We point out that the usual description of interaction by using the optical potential is based on the replacement of nuclei by point-like scatterers. The effects of scattering of the momenta $l \neq 0$, cannot, in principle, be taken into account under this approach. Since this problem has been discussed many times, we present several mathematically rigorous formulas and their proofs on the "physical" level of rigor and refer to accurate mathematical studies if necessary.

In conclusion we would like to discuss the relation between the low energy scattering ($k \to 0$) on the potentials $U_j(|\mathbf{r} - \mathbf{R}_j|)$ (nuclei) with finite radii of action and point potentials. Seeming contradiction between the scattering of neutrons on the nuclei and the scattering on the system of point potentials consists in the observation that the radius of nuclei forces action is finite and, moreover, has the same order as the scattering length. It leads to the difference of the discrete spectrum of the "physical" nuclei and point potential. But the conclusion that point potentials are "nonphysical" is the mistake.

The contradiction is explained by the fact that in the low energy limit in the scattering on the alone potential the contribution of the s-wave is dominant, moreover two leading terms of the Taylor expansion of the scattering amplitude with respect to k are independent of the nucleus radius r_0:

$$f(\mathbf{kr}) = -a + ika^2 + O(k^2). \tag{3}$$

We will show below that for point potential two leading terms of the Taylor expansion of the scattering amplitude with respect to k coincide with given above[2]. Hence, point potential is a good approximation for the initial physical problem. Moreover, the problem with point potential is self-adjoint. It is important since we want to check the "losses", we have to choose self-adjoint problem as zero approximation, otherwise we can obtain "parasitic losses", which connected only with the improper choice of the approximation.

Following consideration given above we assume that point potential is the good zero approximation in the problem of the low energy neutron scattering on the nuclei. Actually, the approach based on the point potentials was used in [3, 10].

2. GENERAL FORMULAS OF THE THEORY OF POINT POTENTIALS

For the scattering of a neutron wave with a rather small energy on a ensemble of nuclei, it is natural to replace the nuclei by point-like scatterers, i.e. to replace the potentials U_j in (2) by the perturbations with zero effective radius. Following [4, 10, 3] we call the scattering theory based on the point potentials "Multiple Scattering Theory". One can find the detail discussion of the questions concerning the theory of point potentials, including all formulas of this section, in [4, 10, 14].

In the physical literature, the point-like scatterers are usually modeled by "δ-like" potentials, so that the corresponding Hamiltonian H has the formal form[3] [4, 10]

$$H = H_0 + \sum_j \frac{2\pi\hbar^2}{m}(-F_j)\delta(\mathbf{r} - \mathbf{R}_j), \tag{4}$$

where $H_0 = -\hbar^2/(2m)\Delta$ is the Hamiltonian of a free particle of mass m and the sum is taken over all the positions $\mathbf{R}_j$ of the point-like scatterers. In fact, this formal formula corresponds to the limit[4]of deep spherically symmetric potential wells of small radius r_0 for which the characteristic depth U_0 of the well and the radius are assumed to be related as $U_0\{r_0\} \sim \hbar^2/(2mr_0^2)$ (the braces denote the dependence on a parameter). In the limit as $r_0 \to 0$, the action of each such potential well is characterized only by a single parameter, i.e., the scattering length a_j. We point out that the scattering length a_j is assumed to be constant as $r_0 \to 0$. A specific realization of the passage to the limit from potential wells of constant depth to zero-range potentials is given in Appendix B (see also [14]).

In fact, the "point potentials" are equivalent to the boundary condition

$$\psi|_{|\mathbf{r}-\mathbf{R}_j|\to 0} \to c_j\left[1 - \frac{a_j}{|\mathbf{r} - \mathbf{R}_j|}\right], \tag{5}$$

where c_j are some constants. The bound state in the field of N point-like scatterers corresponding to the energy $E = -\hbar^2\varkappa^2/(2m)$ has the form

$$\psi_E(\mathbf{r}) = \sum_j F_j \frac{e^{-\varkappa|\mathbf{r}-\mathbf{R}_j|}}{|\mathbf{r} - \mathbf{R}_j|}. \tag{6}$$

Similarly, the scattering state corresponding to the incident plane wave with energy $E = \hbar^2k^2/(2m)$ is described as follows:

$$\psi(\mathbf{r};\mathbf{k}) = \exp(i\mathbf{k}\mathbf{r}) + \sum_j F_j \frac{e^{ik|\mathbf{r}-\mathbf{R}_j|}}{|\mathbf{r} - \mathbf{R}_j|}. \tag{7}$$

Substituting (6) and (7) into (5), we see that, in the case of bound states, the levels are obtained from the compatibility condition

$$\det Q(i\varkappa) = 0 \tag{8}$$

and, in the case of scattering states, the constants F_j are determined as follows:

$$F_i = -\sum_j Q(k)^{-1}_{ij} \exp(i\mathbf{k}\mathbf{R}_j), \tag{9}$$

where the matrix $Q(k)$ has the form

[2]One can prove analogous results for multiple scatterers when $kr_0 \ll kR \ll 1$ (see e.g. [2])

[3]In a literal sense, this formula is not correct.

[4]In what sense the limit is understood from the mathematical viewpoint is discussed in Appendix A.

$$Q_{ij}(k) = \begin{cases} e^{ik|\mathbf{R}_i - \mathbf{R}_j|}/|\mathbf{R}_i - \mathbf{R}_j|, & i \neq j \\ a_j^{-1} + ik, & i = j. \end{cases} \tag{10}$$

Clearly, in the case of a single scatterer, we have $\varkappa = a^{-1}$ for $a > 0$. For $a < 0$, there are no bound states.

The Green's function of the Hamiltonian (4) (i.e., the integral kernel of the operator $(H - k^2)^{-1}$, $\operatorname{Im} k > 0$) is determined by M. G. Krein's formula for the resolvents

$$G(\mathbf{x}, \mathbf{y}; k) = G_0(\mathbf{x}, \mathbf{y}; k) - \sum_{ij} Q(k)^{-1}_{ij} G_0(\mathbf{x}, \mathbf{R}_i; k) G_0(\mathbf{R}_j, \mathbf{y}; k). \tag{11}$$

Here $G_0(\mathbf{x}, \mathbf{y}; k) = \exp(ik|\mathbf{x} - \mathbf{y}|)/(4\pi|\mathbf{x} - \mathbf{y}|)$ is the free Green's function.

Considering the asymptotics of the wave function as $r \to \infty$, we find the scattering amplitude $F^{(N)}$ at a system of point potentials

$$F^{(N)}(\mathbf{n}; k) = \sum_i F_i e^{-i\mathbf{k}'\mathbf{R}_i} = -\sum_{ij} Q(k)^{-1}_{ij} e^{i\mathbf{k}\mathbf{R}_j - i\mathbf{k}'\mathbf{R}_i}, \qquad \mathbf{k}' = k\mathbf{n}, \quad \mathbf{n} = \mathbf{r}/r. \tag{12}$$

The scattering length $a^{(N)}$ at the system of N centers is determined as

$$a^{(N)} = -F^{(N)}(\mathbf{n}; 0) = \sum_{ij} Q(0)^{-1}_{ij}. \tag{13}$$

3. ONE-CENTER PROBLEM. PASSAGE TO THE ZERO-RANGE POTENTIAL

We consider the scattering of a neutron with small energy at a spherically symmetric potential $U(r)$ with a finite radius r_0 of range (a fixed center) located at the origin. The scattering state $\psi(\mathbf{r}; \mathbf{k})$ is described by the Schrödinger equation

$$-(\hbar^2/(2m))\Delta\psi + U(r)\psi = E\psi, \tag{14}$$

where $\hbar$ is the Planck constant, m is the neutron mass, E is the neutron energy, $\mathbf{k}$ is the wave vector of the incident particle, and $E = \hbar^2 k^2/(2m)$. As $\mathbf{r} \to \infty$, the scattering state satisfies the radiation condition

$$\psi(\mathbf{r}; \mathbf{k}) \to \psi_0(\mathbf{r}; \mathbf{k}) + f(k, \mathbf{n}) e^{ikr}/r, \qquad r \to \infty. \tag{15}$$

The function $\psi_0(\mathbf{r}; \mathbf{k})$ determines the initial state of the particle; to be definite, we assume that $\psi_0(\mathbf{r}; \mathbf{k}) = e^{i\mathbf{k}\mathbf{r}}$.

We consider the original problem in the following limit. We let the radius r_0 of the potential range tend to zero and simultaneously let the depth of the potential well tend to infinity so that the characteristic depth satisfy the relation $U_0(r_0) \sim \hbar^2/(2mr_0^2)$. The last condition implies that, in such a well, there exists a shallow real or virtual level. We pass to the limit so that the energy $E = \pm\hbar^2/(2ma^2)$ of this level remains constant. The quantity a is the so-called "scattering length."

For $kr_0 \ll 1$, the contribution of the momenta $l \neq 0$ to the scattering becomes negligibly small because there exists a centrifugal potential. Hence we consider only the contribution of the s-wave[5]. The wave function taking into account only the scattering of the s-wave and satisfying condition (15) has the form

$$\psi(\mathbf{x}; \mathbf{k}) = e^{i\mathbf{k}\mathbf{r}} + f(k) e^{ikr}/r = 1 + f(k)\,(1/r + ik) + O(r_0) \to c\,(1 - a/r)\,, \quad r_0 \to 0, \tag{16}$$

which implies $f(k) = -a/(1 + ika)$. A pole of the scattering amplitude corresponds to a "shallow" real or virtual level. An example of passing to the "point potential" limit in a sequence of symmetric potential wells of constant depth was considered in Appendix B.

The scattering cross-section is determined as

$$\sigma = 4\pi|f|^2 = (4\pi/k)\operatorname{Im} f(k) = 4\pi a^2/(1 + (ka)^2) \tag{17}$$

[5]The condition that the scattering length a is assumed to be "frozen" as $r_0 \to 0$ is the crucial condition for the last assumption to hold. This condition necessarily cannot be satisfied for the scattering length $\sim r_0$. In this case, the corrections due to the contribution of nonzero momenta $\sim kr_0$ are comparable with the corrections $\sim ka$ that arise in the scattering of the s-wave and are preserved in the scattering amplitude.

4. MANY-CENTER PROBLEM. "ANOMALOUS" BEHAVIOR OF THE SCATTERING LENGTH

In the case of an ensemble of scatterers, it is conventional to replace a_j in formulas (5) and (10) by the scattering length at a *single* point-like scatterer concentrated at a point $\mathbf{R}_j$. But already in the problem of multiple scattering at two centers $\mathbf{R}_1$ and $\mathbf{R}_2$ with scattering lengths a_1 and a_2, this substitution leads to an anomalous behavior of the spectral parameters and the scattering data in the limit as $R = |\mathbf{R}_1 - \mathbf{R}_2| \to 0$. This anomaly, first analyzed in [15] (see also [10]), means that the ground state E_0 in the system of two centers tends to $-\infty$ as $R \to 0$, while the scattering length $a^{(2)}$ tends to 0.

We study this phenomenon in detail. First, we construct the bound states of a system with two centers. Obviously, the desired eigenfunction has the form

$$\Psi_E(\mathbf{r}) = (F_1/|\mathbf{r} - \mathbf{r}_1|)\exp(-\varkappa|\mathbf{r} - \mathbf{r}_1|) + (F_2/|\mathbf{r} - \mathbf{r}_2|)\exp(-\varkappa|\mathbf{r} - \mathbf{r}_2|). \tag{18}$$

Condition (8) leads to the equation

$$(\varkappa - a_1^{-1})(\varkappa - a_2^{-1}) = \exp(-2\varkappa R)R^{-2} \tag{19}$$

It is convenient to analyze the last transcendental equation for the parameter $\varkappa$ starting from graphical considerations. In this case, the left-hand side presents a parabola intersecting the Ox-axis at the points a_1^{-1} and a_2^{-1} and the Oy-axis at the point $(a_1a_2)^{-1}$, while the right-hand side tends monotonically to zero intersecting the Oy-axis at the point R^{-2}.

In the case $a_1,\ a_2 > 0$, Eq. (19) has two positive roots for $a_1a_2 < R^2$ and only one root for $a_1a_2 \geqslant R^2$. In the case where only one of the scattering lengths is greater than zero, there always exists only one positive root. But if $a_1,\ a_2 < 0$, then one positive root exists under the condition that $a_1a_2 > R^2$. We note that the fact that a bound state exists in the system of two centers for $a_1, a_2 < 0$ is an important distinguishing feature of zero-range potentials [4]. Moreover, there are no bound states in the potential of each isolated nucleus.

Thus, for $R < (a_1a_2)^{1/2}$, there always exists a unique negative level $E_0(R)$. Moreover, $E_0(R) \to -\infty$ as $R \to 0$, although it was to be expected that E_0 would tend to the level generated by the point perturbation with the reciprocal scattering length $\left(a^{(2)}\right)^{-1} = a_1^{-1} + a_2^{-1}$ as in the one-dimensional case. Furthermore, it follows from (13) that, in the multiple scattering at two centers, the scattering length is equal to

$$a^{(2)} = R(2a_1a_2 - R(a_1 + a_2))/(a_1a_2 - R^2)\,. \tag{20}$$

In particular, for $a_1 = a_2 = a$, we have $a^{(2)} = 2Ra/(R + a)$. In any case, $a^{(2)}$ tends to 0 as $R \to 0$, but not $a^{(2)} \to a_1a_2/(a_1 + a_2)$ as was to be expected.

To remove this anomaly in the behavior of both the ground state and the scattering length, it is necessary to assume [15] that, for small R, the parameter a_j^{-1} depends on R according to the law $1/a_j(R) = 1/\widetilde{a}_j(R) - 1/R$, where $\widetilde{a}_j(R)$ is a regular function of R with values of the order of the scattering length at an isolated nucleus. After the renormalization, we obtain

$$a^{(2)}(R) \to 4\widetilde{a}_1(0)\widetilde{a}_2(0)/(\widetilde{a}_1(0) + \widetilde{a}_2(0)), \qquad R \to 0. \tag{21}$$

In the case of a large number of centers, we must assume that

$$1/a_j(\rho_j) = 1/\widetilde{a}_j(\rho_j) - \beta_j(\rho_j)/\rho_j\,, \tag{22}$$

where $\rho_j = \min_{i\neq j}|\mathbf{R}_j - \mathbf{R}_i|$ and $\beta_j(\rho_j) \sim 1$ as $\rho_j \to 0$.

In conclusion, we point out that, in the case of several centers, the point potential approximation remains valid for any relations between the scattering lengths at isolated scatterers, the distances between the scatterers, and the wavelengths of incident particles. The only important condition is that the radii of the corresponding potential ranges must be much less than all these three parameters.

But, as the scatterers approach one another and the distance between them becomes comparable with the scattering lengths at isolated nuclei, the meaning of the free parameters in formula (5) becomes different. It is convenient to analyze this effect by studying the bound states. For the bound states, this means that it is necessary to consider the tunneling effects, which become crucial as the scatterers approach one another.

5. HAMILTONIAN OF A NEUTRON IN THE FIELD OF N POINT-LIKE SCATTERERS. THE OPTICAL POTENTIAL.

To derive effective equations describing the repulsion of a neutron from the trap walls in terms of the *optical potential*, we follow the elegant argument presented in [2], where it was first shown that the derivation of equations with pseudopotential is significantly different in the cases of slow $kR \ll 1$ and fast $kR \sim 1$ particles, where R is the characteristic distance between the scatterers. In nuclear physics, the slow particles are associated with to the so-called "ultracold neutrons" $k^{-1} \sim 100\mathring{A}$ and the fast particles are associated with the heat neutrons $k^{-1} \sim 3\mathring{A}$. The pseudopotential for slow particles was first introduced by Ya. B. Zeldovich [8], who also predicted that the neutrons can be stored in material traps.

The introducing the optical potential for slow particles means that the asymptotic behavior of the wave function far from the system of identical point-like scatterers does not change when the scatterers are replaced by the slowly varying potential $u(\mathbf{r}) = 4\pi n(\mathbf{r})a$, where $a_j = a$ is the scattering length. To prove this assertion, we first rewrite formula (9) as follows:

$$e^{i\mathbf{k}\mathbf{R}_i} + \sum_j Q(k)_{ij} F_j = 0\,, \tag{23}$$

or, which is the same,

$$e^{i\mathbf{k}\mathbf{R}_i} + (a_i^{-1} + ik)F_i + 4\pi \sum_{j\neq i} G_0(\mathbf{R}_i, \mathbf{R}_j; k)F_j = 0\,. \tag{24}$$

We denote the "neutron amplitudes" by $\Psi_i = -F_i/a_i$ and, for simplicity, assume that $a_i = a$ is independent of i. Then

$$\Psi_i = \psi_0(\mathbf{R}_i; \mathbf{k}) - ika\Psi_i - 4\pi a \sum_{j\neq i} G_0(\mathbf{R}_i, \mathbf{R}_j; k)\Psi_j. \tag{25}$$

We point out that formula (25) is obtained from (9) by *identical transformations*. For further simplifications, in the right-hand side of the last formula, we replace the sum by an integral under the condition that $k \ll R^{-1}$. In this case, the coefficients $G_0(\mathbf{R}_i, \mathbf{R}_j; k)$ vary slowly with j (the Zeldovich case). We note that $ik = 4\pi \lim_{r\to 0} \operatorname{Im} G(\mathbf{R}_i, \mathbf{R}_i + \mathbf{r}; k)$, i.e., we can assume that only the real part of the continuation of $G(\mathbf{R}_i, \mathbf{R}_i; k)$ for $j = i$ is "absent" in the sum. Replacing the neutron amplitudes Ψ_i by a continuous function $\Psi(\mathbf{r})$, $\Psi(\mathbf{R}_i) = \Psi_i$, varying at distances $\sim k^{-1}$, we pass from the sum to an integral in the last formula:

$$\Psi(\mathbf{r}) = \psi_0(\mathbf{r}; \mathbf{k}) - 4\pi a \int d^3\mathbf{r}' n(\mathbf{r}') G_0(\mathbf{r}, \mathbf{r}'; k)\Psi(\mathbf{r}'), \tag{26}$$

where $n(\mathbf{r})$ is the density of scatterers[6]. The integral around the center $\mathbf{R}_j = \mathbf{R}_i$ is small under the condition that $a \ll R$:

$$4\pi a \int_{|\mathbf{r}'-\mathbf{r}|<R} d^3\mathbf{r}' n(\mathbf{r}') G_0(\mathbf{r}, \mathbf{r}'; k)\Psi(\mathbf{r}') \sim aR^2/R^3 \sim a/R. \tag{27}$$

Equation (26) is equivalent to the differential Schrödinger equation:

$$-\Delta\Psi(\mathbf{r}) + u(\mathbf{r})\Psi(\mathbf{r}) = k^2\Psi(\mathbf{r}), \qquad u(\mathbf{r}) = 4\pi n(\mathbf{r})a. \tag{28}$$

Here $u(\mathbf{r})$ is the so-called *optical potential* (the Fermi pseudopotential). Solving Eq. (28) with pseudopotential is, in fact, equivalent to calculating the inverse of the matrix Q_{ij} in (10).

Far from matter, i.e., in the domain $|\mathbf{r}-\mathbf{R}_j| \gg k^{-1}$, the Green's function $G(\mathbf{R}_j, \mathbf{r}; k)$ is a smooth function. Hence Eq. (7) in this domain can be written in integral form

$$\psi(\mathbf{r}; \mathbf{k}) = \psi_0(\mathbf{r}; \mathbf{k}) - 4\pi a \int d^3\mathbf{r}' n(\mathbf{r}') G_0(\mathbf{r}', \mathbf{r}; k)\Psi(\mathbf{r}'). \tag{29}$$

Since Eqs. (26) and (29) coincide, the neutron wave function $\psi(\mathbf{r}; \mathbf{k})$ outside matter must be identified with the function[7] $\Psi(\mathbf{r})$.

Under the assumption that the amplitudes Ψ_i vary slowly with the number i, we can replace the sum by an integral also in formula (12) determining the scattering amplitude $F^{(N)}$. Thus, we obtain

[6] As usual, we assume that the volume $d^3\mathbf{r}$ contains $n(\mathbf{r})d^3\mathbf{r}$ scatterers.

[7] Strictly speaking, Eq. (26) holds only inside matter; it can be "continued" to the entire space only under some additional conditions.

$$F^{(N)}(\mathbf{n};k)=\sum_i F_i e^{-i\mathbf{k}'\mathbf{R}_i}=-\int d^3\mathbf{r}'e^{-i\mathbf{k}'\mathbf{r}'}an(\mathbf{r}')\psi(\mathbf{r}')=-\frac{1}{4\pi}\langle\psi_0(\mathbf{k}')|u|\Psi\rangle, \tag{30}$$

which completely agrees with the general formula for the scattering amplitude at a finite-range potential.

In conclusion, we note that in [5] the neutron amplitudes are defined as $\Psi_i=-(a_i^{-1}+ik)F_i$. Acting as above, we obtain the following equation for the smoothed amplitudes $\Psi(\mathbf{r})$:

$$-\Delta\Psi(\mathbf{r})+\widetilde{u}(\mathbf{r})\Psi(\mathbf{r})=k^2\Psi(\mathbf{r}),\qquad \widetilde{u}(\mathbf{r})=4\pi n(\mathbf{r})(a/(1+ika)). \tag{31}$$

The optical potential in the last formula contains an imaginary correction. But, the existence problem concerning the imaginary additional term in the optical potential cannot be solved on the same level of rigor as Eqs. (28) and (31) were obtained.

6. RANDOM SCATTERING LENGTH

Apparently, the optical potential describes well the case of an ideal infinite crystal for which all the scattering lengths are assumed to be the same. In fact, as was shown in Section 4, the scattering length at the jth center depends on the position of all the other scatterers. Thus, it can be somewhat different even for identical nuclei because of various defects of the lattice, far distances from the matter boundary, heat oscillations of nuclei, the absence of higher-order terms, etc. In any case, the "characteristic difference" between the scattering length in matter and the scattering length at an isolated nucleus is of order $1/R$. Here we consider the simplest model in which all the scattering lengths are assumed to be random variables. In this case, the positions $\mathbf{R}_j$ of the scatterers are assumed to be fixed. Such a model allows one to introduce a random element and, at the same time, to perform simple analytic calculations.

We make the following model assumption: let the reciprocal of the scattering length $\alpha_j=a_j^{-1}$ be a Lorentz distributed random variable with half-width $\bar{\alpha}_j$. We readily note that the "drawback" of such a distribution is that the scattering length itself does not have any mean value, since the integral

$$\frac{1}{\pi}\int_{-\infty}^{\infty}\frac{1}{\bar{\alpha}+\tau}\left(\frac{\varkappa}{\tau^2+\varkappa^2}\right)d\tau \tag{32}$$

diverges near the point $\tau=-\bar{\alpha}$ like the integral $\int dx/x$ at zero. But the mean value of the scattering amplitude exists and can be determined as the integral

$$\bar{f}(k)=-\frac{1}{\pi}\int_{-\infty}^{\infty}\frac{1}{\bar{\alpha}+\tau+ik}\left(\frac{\varkappa}{\tau^2+\varkappa^2}\right)d\tau=\frac{1}{\bar{\alpha}+i\varkappa+ik}, \tag{33}$$

which can elementary be calculated by using the residue technique. It is easily seen that the mean scattering cross-section is

$$\bar{\sigma}=(4\pi/k)\operatorname{Im}\bar{f}(E)=((4\pi a^2)/(1+(k+\varkappa)^2a^2))(1+\varkappa/k). \tag{34}$$

Now we consider the case of many scatterers. According to (7) and (9), the scattering state is determined as follows:

$$\psi(\mathbf{r};\mathbf{k})=\psi_0(\mathbf{r};\mathbf{k})-\sum_{ij}Q(k)^{-1}_{ij}\frac{e^{ik|\mathbf{r}-\mathbf{R}_i|}}{|\mathbf{r}-\mathbf{R}_i|}\psi_0(\mathbf{R}_j;\mathbf{k}), \tag{35}$$

where the diagonal entries of the matrix Q are $\bar{\alpha}_j+\tau_j$ and τ_j are independent random variables. We introduce the scattering state averaged over all the realizations of these variables:

$$\langle\psi(\mathbf{r};\mathbf{k})\rangle=\psi_0(\mathbf{r};\mathbf{k})-\sum_{ij}\langle Q(k)^{-1}_{ij}\rangle\frac{e^{ik|\mathbf{r}-\mathbf{R}_i|}}{|\mathbf{r}-\mathbf{R}_i|}\psi_0(\mathbf{R}_j;\mathbf{k}) \tag{36}$$

To find the entries $\langle Q(k)^{-1}_{ij}\rangle$ of the averaged matrix, we use the so-called "supersymmetric trick" [6, 7, 16]. According to the general scheme, we introduce commuting (complex) variables z_i and the anticommuting (Grassmannian) variables θ_i; then $Q(k)^{-1}$ can be calculated by using the so-called Berezin integral

$$[4\pi\widehat{G}_0(i',j';k)+(\bar{\alpha}_{i'}+\tau_{i'})\delta_{i'j'}]^{-1}_{i,j}=i\int z_i^*z_j\exp\left[i\sum_{i',j'}(z^*_{i'}z_{j'}+\theta^*_{i'}\theta_{j'})4\pi\widehat{G}_0(i',j';k)\right.$$
$$\left.+i\sum_{i'}(z^*_{i'}z_{i'}+\theta^*_{i'}\theta_{i'})(\bar{\alpha}_{i'}+\tau_{i'})\right]DzD\theta\,, \tag{37}$$

where

$$\widehat{G}_0(i,j;k)=\begin{cases}G_0(\mathbf{R}_i,\mathbf{R}_j;k), & i\neq j,\\ ik/(4\pi), & i=j,\end{cases}\qquad Dz=\prod_i z_i^*z_i\,,\quad D\theta=\prod_i\theta_i^*\theta_i\,.$$

Let p_i be the distribution density of the random variable τ_i, and let g_i be the characteristic function of this density:

$$g_i(x)=\int_{-\infty}^{\infty}e^{itx}p_i(t)\,dt\,.$$

Averaging (37) and taking into account the fact that τ_i are independent, we obtain

$$\langle[4\pi\widehat{G}_0(i',j';k)+(\bar{\alpha}_{i'}+\tau_{i'})\delta_{i'j'}]^{-1}_{i,j}\rangle=i\int z_i^*z_j\exp\left[i\sum_{i',j'}(z^*_{i'}z_{j'}+\theta^*_{i'}\theta_{j'})4\pi\widehat{G}_0(i',j';k)\right.$$
$$\left.+i\sum_{i'}(z^*_{i'}z_{i'}+\theta^*_{i'}\theta_{i'})\bar{\alpha}_{i'}\right]\prod_{i'}g_{i'}(z^*_{i'}z_{i'}+\theta^*_{i'}\theta_{i'})\,DzD\theta\,. \tag{38}$$

The integral in (38) is finite if τ_i are Lorentz distributed:

$$p_i(t)=\frac{1}{\pi}\frac{\varkappa_i}{t^2+\varkappa_i^2}\,,\qquad \varkappa_i>0\,. \tag{39}$$

In this case, the characteristic function has the form

$$g_i(x)=\exp(-\varkappa_i|x|)\,, \tag{40}$$

and we obtain the following finite expression for the integral in (38):

$$\langle[4\pi\widehat{G}_0(i',j';k)+(\bar{\alpha}_{i'}+\tau_{i'})\delta_{i'j'}]^{-1}_{i,j}\rangle=i\int z_i^*z_j\exp\left[i\sum_{i',j'}(z^*_{i'}z_{j'}+\theta^*_{i'}\theta_{j'})4\pi\widehat{G}_0(i',j';k)\right.$$
$$\left.+i\sum_{i'}(z^*_{i'}z_{i'}+\theta^*_{i'}\theta_{i'})(\bar{\alpha}_{i'}+i\varkappa_{i'})\right]DzD\theta=\left[4\pi\widehat{G}_0(i',j';k)+(\bar{\alpha}_{i'}+i\varkappa_{i'})\delta_{i'j'}\right]^{-1}_{i,j}\,. \tag{41}$$

In the case of a single scattering center, this procedure implies (33). Thus, the averaging over the scattering state realizations has the form

$$\langle\psi(\mathbf{r};\mathbf{k})\rangle=\psi_0(\mathbf{r};\mathbf{k})-\sum_{i,j}\left[\widehat{G}_0(i',j';k)+(\bar{\alpha}_{i'}+i\varkappa_{i'})\delta_{i'j'}\right]^{-1}_{i,j}\psi_0(\mathbf{R}_i;\mathbf{k})G_0(\mathbf{R}_j,\mathbf{r};k)\,. \tag{42}$$

Following the argument given in Section 1, for the case in which $\bar{\alpha}_i=\bar{\alpha}\sim a^{-1}$ and $\varkappa_i=\varkappa\sim R^{-1}$, we obtain the following equation for the "smoothed" neutron amplitudes:

$$-\Delta\Psi(\mathbf{r})+u(\mathbf{r})\Psi(x)=k^2\Psi(\mathbf{r}),\qquad u(\mathbf{r})=4\pi n(\mathbf{r})(\bar{\alpha}+i\varkappa)^{-1}, \tag{43}$$

where $\Psi(\mathbf{r})$ coincides with $\langle\psi(\mathbf{r};\mathbf{k})\rangle$ for sufficiently large r.

7. CONCLUSION

In this paper, we analyzed the "optical potential" method for describing the interaction of slow neutrons with the medium. We showed that the well-known formulas of the theory of multiple scattering of waves corresponds to the limit of the so-called "zero-range" potentials, which are three-dimensional analogs of δ-potentials.

We pass to the optical potential under the assumption that the "neutron amplitudes" vary slowly at distances of the order of the distance between the scatterers and the scattering lengths are the same for all the centers and coincide with the scattering lengths at isolated nuclei.

But already in the problem with two scattering centers, the assumption that the scattering lengths are equal to the scattering length at an isolated center leads to an "anomalous" behavior of the scattering data in the limit as $R\to 0$. The situation can be "improved" by using a "renormalization" of the scattering lengths. The renormalization is reduced to the change $a_j^{-1}\to\widetilde{a}_j(R)^{-1}-R^{-1}$.

A similar renormalization can be justified "heuristically" in the case of many scatterers. In this case, it is reduced to the change $a_j^{-1} \to \widetilde{a}_j(R)^{-1} - \beta_j(R)R^{-1}$, where R is the minimal distance between the scatterers.

We assume that, in a real situation when the crystal nonideality, the boundary existence, and the heat motion of nuclei are taken into account, the function $\beta_j(R)$ can be assumed to be a random variable. This assumption lead to an indeterminacy in the reciprocal scattering length $\sim R^{-1}$. In this case, it is natural to obtain the "averaged" description of the scattering process. But, in the general case, the process of obtaining constructive formulas is a technically complex procedure because it is necessary to invert the matrix (10). To overcome this difficulty, we assume that the random variables are Lorentz distributed and obtain the averaged optical potential explicitly, using the so-called "supersymmetric trick" [6]. The averaged optical potential turns out to be dissipative, and the imaginary correction to it coincides with the parameter of the Lorentz distribution.

8. ACKNOWLEDGMENTS.

The authors with to express their gratitude to A. Barabanov, R. Golub, and E. Korobkina for stimulating discussions. This research was supported by INTAS under grant no. 00-257 and by DFG–RAS project no. DFG 436 RUS 113/572.

9. APPENDIX A

Unfortunately, formula (4) does not give a mathematically well-defined Hamiltonian H for any choice of the nonzero coupling constants $c_j = -2\pi\hbar^2 m^{-1} F_j$. This originates from the fact that, in contrast to the one-dimensional case, the quadratic form $f \mapsto \langle H_0 f \mid f\rangle + \sum_j c_j |f(\mathbf{R}_j)|^2$, well-defined on the space of finite functions $C_0^\infty(\mathbb{R}^3)$, cannot be continued to a closed quadratic form in $L^2(\mathbb{R}^3)$ in all dimensions greater than unity [15]. Intuitively, we see that the most natural method for overcoming this difficulty is to consider the Hamiltonian H as the limit of a family of Hamiltonians of the form

$$H_\varepsilon = H_0 + \sum_j c_j^{(\varepsilon)} V_\varepsilon(\mathbf{x} - \mathbf{R}_j)\,, \tag{44}$$

where $V_\varepsilon(\mathbf{x})$ are "regular" functions tending to the Dirac function $\delta(\mathbf{x})$ as $\varepsilon \to 0$, while the form of the coupling constants $c_j^{(\varepsilon)}$ must be determined so that H_ε converge to H in some operator topology. In this context, the topology of uniform resolvent convergence is the strongest topology. Namely, the family H_ε converges in this topology to H as $\varepsilon \to 0$ if the family $(H_\varepsilon - z)^{-1}$ converges to $(H - z)^{-1}$ in the operator norm for some (and hence for any) nonreal $z \in \mathbb{C}$.

If we want to obtain a nontrivial limit in a neighborhood of the point $\mathbf{R}_j$ (i.e., an operator H whose action on the functions concentrated in a sufficiently small neighborhood of the point $\mathbf{R}_j$ is other than H_0), then it is necessary that $c_j^{(\varepsilon)}$ be nonnegative for sufficiently small $\varepsilon > 0$ and do not exceed ε in the order of magnitude [4]. Intuitively, this means that the potential $c_j\delta(\mathbf{r} - \mathbf{R}_j)$ in formula (4) must be an attracting potential with an infinitely small coupling constant c_j.

10. APPENDIX B

We consider a spherically symmetric potential well of constant depth U_0 and radius r_0. In such a potential well, we seek bound states with energy $E = -\hbar^2\varkappa^2/(2m)$ and momentum $l = 0$. As usual, we introduce an eigenfunction in the form $\chi(r)/r$ and obtain

$$\chi = \begin{cases} A\sin(\varkappa' r), & r < r_0, \\ B\exp(-\varkappa r), & r \geqslant r_0, \end{cases} \tag{45}$$

where we use the notation $(\varkappa')^2 = 2mU_0/\hbar^2 - \varkappa^2$. Equating the logarithmic derivatives χ'/χ at the point $r = r_0$, we obtain the following system of equations:

$$\eta = -\xi\cot\xi, \quad \xi^2 + \eta^2 = u_0, \tag{46}$$

where $\xi = \varkappa' r_0$, $\eta = \varkappa r_0$, and $u_0 = 2mr_0^2 U_0/\hbar^2$. Graphically, the solutions of this system are the points at which the circle of radius[8] u_0 intersects the curves $\eta = -\xi \cot \xi$. Clearly, the positive solutions ξ and η exist if the radius u_0 is greater than $\pi/2$. The parameter η determines the "depth" of the level. Now we fix the level energy and let the radius of the well tend to zero. In this case, the level becomes "shallow," i.e., $\eta \to 0$. Solving system (46) by the perturbation theory method in the parameter η, we obtain $\xi = \pi\,(n + 1/2) + \eta/(\pi(n + 1/2)) + O(\eta^2)$ and $u_0 = \pi^2\,(n + 1/2)^2 + 2\eta + O(\eta^2) = \pi^2\,(n + 1/2)^2 + 2r_0/a + O((r_0/a)^2)$, where $a = \varkappa^{-1}$ is the scattering length. This gives the formula for the sequence of potentials $U_0\{r_0\}$, $r_0 \to 0$, with a fixed scattering length:

$$U_0\{r_0\} = \frac{\hbar^2}{2mr_0^2}\left[\pi^2\left(n + \frac{1}{2}\right)^2 + \frac{2r_0}{a} + O\left(\frac{r_0}{a}\right)^2\right]. \tag{47}$$

The potential wells U_0 become deep as $r_0 \to 0$, but they are "weaker" than the δ-sequence (the sequence tending to the δ-function). This can easily be seen if we write the characteristic depth of the well in the form

$$\frac{\hbar^2}{2mr_0^2} = \frac{2\pi\hbar^2 r_0}{3m}\delta\{r_0\}, \qquad \delta\{r_0\} = \frac{1}{\Omega(r_0)}, \tag{48}$$

where $\Omega(r_0) = 4\pi r_0^3/3$ is the volume of a sphere of radius r_0 and the sequence $\delta\{r_0\} \to \delta(\mathbf{r})$ as $r_0 \to 0$. Clearly, the coefficient of $\delta\{r_0\}$ (the "coupling constant") tends to zero as $r_0 \to 0$.

REFERENCES

1. E. Korobkina, R. Golub, J. Butterworth, P. Geltenbort, and S. Arzumanov, "Temperature Dependence of Ultracold Neutron Loss Rates," Physical Review. B **70**, 035409 (2004).
2. A. L. Barabanov and S. T. Belyaev, "Potential of Ultra-Cold Neutron Interaction with Matter," Fiz. Atomn. Yadra **62** (5), 824–831 (1999) [Physics of Atomic Nuclei **62** (5), 69–775 (1999)].
3. V. K. Ignatovich, "Ultracold Neutrons — Discovery and Research," Usp. Fiz. Nauk **166** (3), 303–326 (1996) [Phys. Usp. **39** (3), 283–304 (1996)].
4. A. I. Baz', Y. B. Zeldovich, and A. M. Perelomov, *Scattering, Reactions and Decay in Nonrelativistic Quantum Mechanics* (Nauka, Moscow, 1971; Israel Program for Scientific Translations, Jerusalem, 1969).
5. I. M. Lifshitz, S. A. Gredeskul, and L. A. Pastur, *Introduction to the Theory of Disordered Systems* (Nauka, Moscow, 1982).
6. E. Brézin, D. J. Gross, and C. Itzykson, "Density of States in the Presence of a Strong Magnetic Field and Random Impurities," *Nuclear Physics. B.* **235** [FS11], 24–44 (1984).
7. K. B. Efetov, "Supersymmetry and Theory of Disordered Metals," *Advances in Physics.* V. **32** (1983), 53–127.
8. Ya. B. Zeldovich, Zh. Exper. Teoret. Fiz. **36**, 1952 (1959) [Sov. Physics JETP **9**, 1389 (1959)].
9. L. L. Foldy, "The Multiple Scattering of Waves," Phys. Rev. **67**, 107–119 (1945).
10. Y. N. Demkov and V. N. Ostrovsky, *Zero-Range Potential Method in Atomic Physics* (Izd-vo LGU, Leningrad, 1975; Plenum, New York, 1988).
11. A. L. Barabanov and S. T. Belyaev "Ultracold Neutrons Escape from Material Trap: Theory for Coherent Inelastic Scattering," Preprint arXiv:nucl-th/0409055.
12. V. K. Ignatovich, *The Physics of Ultracold Neutrons* (Nauka, Moscow, 1986; Clarendon, Oxford, 1990).
13. V. K. Ignatovich, "Dynamical Diffraction," Preprint arXiv:physics/0404009.
14. S. Albeverio, F. Gesztesy, R. Høegh-Krohn, and H. Holden, *Solvable Models in Quantum Mechanics* (Springer, New York–Berlin, 1988).
15. T. K. Rebane and R. I. Sharibdzhanov, "Magnetic Properties of the Simplest Systems in the Zero-Range Potential Model," Teoret. i Eksperim. Khim. **10**, 444–449 (1974).
16. G. Parisi, "An Introduction to the Statistical Mechanics of Amorphous Systems," in *Les Houches Session XXXIX on Recent Advances in Field Theory and Statistical Mechanics* (North-Holland, Amsterdam–New York, 1984), pp. 473–523.
17. M. Reed and B. Simon. *Methods of Modern Mathematical Physics*, Vol. II (Acad. Press, New York, 1975).

[8]The necessity of the condition $u_0 \sim 1$ for the level existence follows from the indeterminacy principle.