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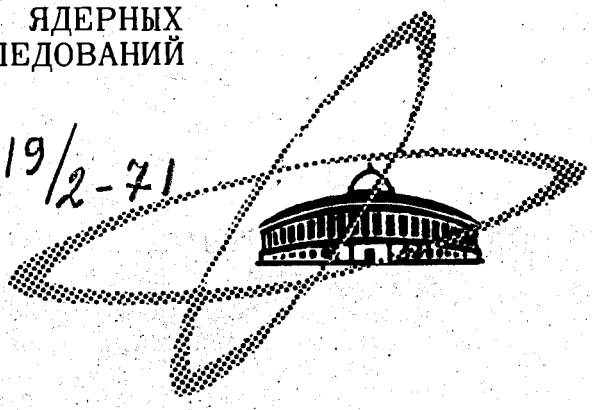

E4 - 6095

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ESTIMATE OF UPPER AND LOWER BOUNDS TO CHARACTERISTICS OF TWO- AND THREE-BODY SYSTEMS

ЛАБОРАТОРИЯ ТЕОРЕТИЧЕСКОЙ ФИЗИКИ

1971

E4 - 6095

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ESTIMATE OF UPPER AND LOWER BOUNDS TO CHARACTERISTICS OF TWO- AND THREE-BODY SYSTEMS

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In this paper we will talk about deriving upper and lower bounds to the binding energy and scattering lengths in the two-nucleon system and to the tritium binding energy, as well. Here both the upper and lower bounds are obtained by solving the dynamical equations without using the trial functions, apriori form.

To obtain good estimates of the upper and lower bounds is of a special importance for the problem of three and more nucleons because the direct solution of the corresponding equations with present realistic local potentials even for the systems with negative total energy proves to be a rather bulky problem.

To estimate the lower bound to the binding energy of three-body system a number of procedures[1] has been proposed. Of these the most successfull is probably the procedure given by Fabri and Fiorio, which is the iteration process in the differential formulation. The difference between the upper and lower values of the binding energy for the spinless three-body system (for the Gaussian potential) calculated by these authors, equals fractions of percent of the energy. However, for the potentials singular at

zero the method is expected to be not so effective. Estimates of tritium binding energy for more realistic potentials, calculated recently[2] by a method proposed by Hall and Post, also do not give the good lower bound in a number of cases.

We will look for the lower (and upper, as well) bound to the binding energy basing on the following: let us have the exact Hamiltonian of a system H and an approximate Hamiltonian $\tilde{H}$, then if $H \leq \tilde{H}$ or $H \geq \tilde{H}$,[x] the spectra of both operators satisfy the same inequalities[3]. Thus, the problem now consists in finding sufficiently effective procedure for $\tilde{H}$, or in other words the approximate interaction potential, to be constructed. In what follows we will consider the attractive potentials only, for which the given above theorem holds (a generalization to the arbitrary form potentials is not difficult). For simplicity we restrict ourselves to the S-state over the relative motion of particle pairs.

Thus, let us have the pair short-range potential $\langle k|V|k'\rangle$. Now introduce the approximate potential by means of the Bateman formula[4]:

$$\langle k|V_B^N|k'\rangle = \sum_{i,l}^{N} [d^{-1}]_{il} \langle k|V|i\rangle\langle j|V|k'\rangle, \qquad (1)$$

where $d_{il} = \langle i|V|j\rangle$, $|i\rangle$ – the S-harmonic of the plane wave with the momentum S_i. It is easy to see[5] that $V \leq V_B^N$ (1A) for any N; really, we have

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[x] Operator inequalities are usually understood in the sense that $H \leq H_1$ means $\langle\psi|H|\psi\rangle \leq \langle\psi|H_1|\psi\rangle$, where $|\psi\rangle$ is a function from the definition region of the operators H and H_1.

$$(\langle\psi| + \sum_i C_i^* \langle i|)V(\sum_j C_j |j\rangle + |\psi\rangle) \leq 0 \qquad (2)$$

for the attractive potential V. Here $|\psi\rangle$ is an arbitrary function, for example, the plane wave $|k\rangle$. By minimizing (2) with respect to C_i and calculating (2) at values C_i, which provide the minimum of (2), we get that $V < V_B^N$, where V_B^N is defined by the formula (1). The equality in the condition (1A) takes place if k or k' are equal to S_i.

So, the calculation with the factorized potential (1) will give the upper bound to the energy of particles interacting with each other through the potential V. The difference from the energy upper bound found by using the variational trial functions, as we see, is that the expression (1) does not involve any apriori assumption about a shape of the system trial functions and the functions themselves are obtained as solutions of the corresponding dynamical equations. Because of V^N is tending uniformly to V as N increases[6], the solutions of equations with "intermediate"[7] Hamiltonians H^N will approach the exact solution.

Now let us find the lower bound to the binding energy of deuteron and tritium. To this end, as was mentioned above, the "intermediate" Hamiltonians $\tilde{H}^N$ which always are smaller than the exact ones H, must be derived, or, equivalently, it is necessary to obtain $\tilde{V}^N \leq V$ (3). Since the potentials are attractive, the relation (3) is equivalent to the condition $|\tilde{V}^N| \geq |V|$. We have:

$$|V(k,k')| \equiv |V_B^N(k,k')| + [|V(k,k')| - |V_B^N(k,k')|] \equiv$$

$$\equiv |V_B^N(k,k')| + V_1(k,k') \leq |V_B^N(k,k')| + |V_1(k,k')|.$$

Taking account of the property (1A) for V_1 we have

$$V_1(k,k) \geq 0. \tag{4}$$

Next, let us demonstrate that the inequality[x/]

$$|V_1(k,k')| \leq \sqrt{V_1(k,k)V_1(k',k')} \tag{5}$$

holds. We rewrite (1) in the form:

$$V_B^N(k,k') = \langle k|V|p\rangle\langle p|d^{-1}|q\rangle\langle q|V|k'\rangle,$$

where $|p\rangle$ and $|q\rangle$ are the N-dimensional vectors. Then

$$V_1(k,k') = \langle k|V|k'\rangle - \langle k|V|p\rangle\langle p|d^{-1}|q\rangle\langle q|V|k'\rangle$$
$$= \langle k|(V - V|p\rangle\langle p|d^{-1}|q\rangle\langle q|V)|k'\rangle.$$

Due to (4) the operator in parenthesis is positive definite, therefore it is possible to introduce the positive definite operator $\hat{R}$ and vectors x and y in Hilbert space via the equalities

$$\hat{R} \equiv (V - V|p\rangle\langle p|d^{-1}|q\rangle\langle q|V)^{1/2}$$
$$x \equiv \hat{R}|k\rangle$$
$$y \equiv \hat{R}|k'\rangle$$

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x/ The inequality (5) for the local potential $V(k,k')$ can easily be derived by using the known inequality of Helder $\int|f(x)g(x)|dx \leq \sqrt{\int f^2(x)dx}\sqrt{\int g^2(x)dx}$ and integral representation for the partial harmonic of local potential V. In this way, (5) applied directly to the local potential, can be used for obtaining the energy lower bound.

in such a way that $V_1(k,k') = (x,y)$ – is the scalar product. But for the scalar product of two vectors in the Hilbert space we have $|(x,y)| \leq \sqrt{(x,x)(y,y)}$ thus the inequality (5) is proved.

Now we introduce the approximate potential through the formula:

$$\tilde{V}^N(k,k') = -[|V_B^N(k,k')| + \sqrt{[|V(k,k)| - |V_B^N(k,k)|][|V(k',k')| - |V_B^N(k',k')|]}. \quad (6)$$

It possesses the following properties:

(1) $\tilde{V}^N(k,k) = V(k,k)$

(2) $\tilde{V}^N(k,i) = V(k,i)$, $\tilde{V}^N(i,k') = V(i,k')$

(3) $\tilde{V}^N \leq V$.

The latter property guaranties the lower bound for the system energy to be found. It may be expected that due to the additional condition (1), the potential (6) is closer to the exact one than (1) for which the condition (2) is only fulfilled. It should be noted also that the latter inequality holds for the nondiagonal matrix elements (for diagonal matrix elements, because of (1) the equality takes place.

Next, it is clear that the potentials (1) and (6) provide also the possibility for the upper and lower bounds to the nucleon-nucleon scattering lengths to be found. Indeed, let in the two-body system one level ϵ be close to zero, then taking in a t-matrix the pole term only, we have

$$a \sim t(k = k' = Z = 0) \sim \frac{1}{\epsilon}$$

i.e. the upper and lower bounds to ϵ represent the estimate of those to the scattering length.

Using as starting ones the potentials in the form of exponent and Gaussian functions, we have carried out for the approximate potential (6) the calculations of singlet and triplet scattering lengths, binding energy of deuteron and tritium. The tritium binding energy was found by solving the Faddeev equations system with t- matrices constructed with the potential (6). Results are listed in Table.

In the calculations the following values of the potential parameters were used:

$$V_0^s = -32.348\ fm^{-2}$$
$$\alpha^s = 0.315\ fm^{-2}$$
$$V_0^t = -77.022\ fm^{-2} \qquad r_s = 2.704\ fm$$
$$\alpha^t = 0.480\ fm^{-2} \qquad r_t = 1.749\ fm$$
$$V^s = -103.343\ fm^{-2}$$
$$\beta^s = 1.364\ fm^{-2}$$
$$V^t = -179.249\ fm^{-2}$$
$$\beta^t = 1.442\ fm^{-2}$$

The resulting calculations with the potential (1) are taken from the work /8/ in which the value $N=4$ had been used.

The potential (6) was computed with $N=3$, the cuts being found from the condition of $\min \chi^2$, where

$$\chi^2 = \frac{\int [V(k,k') - \tilde{V}^{(3)}(k,k')]^2 dk\,dk'}{\int V^2(k,k')\,dk\,dk'}$$

In all the cases $\chi^2 \sim 10^{-3}$. As is seen from Table, the relative value of the distance between the upper and lower bounds does not exceed 5% at worst.

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Received by Publishing Department
on October 22, 1971.

T a b l e

Type of potential		Singlet scattering length a_s (fm)	Triplet scattering length a_t (fm)	Binding energy of deuteron (MeV)	Binding energy of tritium (MeV)
exact	approximate				
	(1)	-23.6	5.450	2.20	8.96
$V_0 e^{-\alpha r^2}$	(6)	-25	5.424	2.30	9.02
$V_0 e^{-\beta r}$	(1)	-23.6	5.450	2.20	9.220
	(6)	-25.4	5.33	2.40	9.227