ON THE USE OF FADDEEV EQUATIONS FOR CALCULATING THE ELECTRON SCATTERING LENGTH ON HYDROGEN

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Abstract

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ON THE USE OF FADDEEV EQUATIONS FOR CALCULATING THE ELECTRON SCATTERING LENGTH ON HYDROGEN

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Recently, a line of work has been developing that is connected with the application of Faddeev equations for the three-particle scattering matrix ([1]) to atomic problems (see, for example, ([2–4])). Interesting results were obtained in ([3]) for the scattering of slow electrons by the hydrogen atom. For the even amplitudes the authors used a separable expansion (the Hilbert–Schmidt expansion). This leads to an infinite system of Fredholm-type integral equations for the coefficients of the expansion of the exact amplitude in the eigenfunctions of the kernel of the two-particle scattering problem. Retaining a finite number of terms in the separable expansion of the even amplitudes cuts off this system. For $L = 0$ (L is the total angular momentum of the three particles), the energy of the bound state (the ion H^-) and the position of resonances in the elastic region were calculated. It turned out that the separable series in this problem converges rapidly, and already the first 2–3 terms give good quantitative agreement (within several percent) with experiment and with variational calculations.

It seems of interest to us to investigate the convergence of the separable expansion for the scattering amplitude, and not only for the problem of calculating bound and resonant states. The position of bound states is determined by the zeros of the determinant of the system of integral equations, whereas the amplitude is equally sensitive to the magnitude of the "numerator." If the convergence here also proved to be sufficiently rapid, this would give hope that the method could be applied to a very broad class of problems in atomic physics, for example to the scattering of slow electrons by alkali metals. In the present note we present the results of calculations of the singlet and triplet scattering lengths on the ground state of the hydrogen atom.

The formula for the total elastic-scattering cross section (for electron energy tending to zero) has the form

$$\sigma = \pi^5 \left\{ \frac{1}{4} \left| \chi_{10}^{(1)}(0) + \chi_{10}^{(2)}(0) \right|^2 + \frac{3}{4} \left| \chi_{10}^{(1)}(0) - \chi_{10}^{(2)}(0) \right|^2 \right\}. \quad (1)$$

The quantities $\chi_{10}^{(i)}(0)$ are determined from the solution of a system of integral equations analogous to system (3.14) of ([3]):

$$\chi_{nl}^{(i)}(q) = \eta_{nl}^{(i)}(q) + \sum_{j \neq i}^{3} \sum_{n'l'} \int_0^\infty dq' \, q'^2 \, K_{nl,n'l'}^{ij}(q,q') \chi_{n'l'}^{(j)}(q'), \quad i = 1,2,3. \quad (2)$$

The kernels $K_{nl,n'l'}^{ij}$ and the free term $\eta_{nl}^{(i)}$ are known, although very cumbersome, functions. The kernels have the following properties:

$$\begin{aligned} K_{nl,n'l'}^{12}(q;q') &= K_{nl,n'l'}^{21}(q;q'), \\ K_{nl,n'l'}^{13}(q;q') &= (-1)^{l+l'} K_{nl,n'l'}^{23}(q;q'), \\ K_{nl,n'l'}^{31}(q;q') &= (-1)^{l+l'} K_{nl,n'l'}^{32}(q;q'). \end{aligned} \quad (3)$$

These properties make it possible to transform system (2) into a system for the functions $\chi_{nl}^{(+)} = \chi_{nl}^{(1)} + \chi_{nl}^{(2)}$, $\chi_{nl}^{(-)} = \chi_{nl}^{(1)} - \chi_{nl}^{(2)}$, and $\chi_{nl}^{(3)}$*.

Formula (2) was obtained with the aid of the separable expansion of the pair amplitudes entering as kernels in the original Faddeev equations ([3,4]):

$$t_l^{(i)}(p_i;p_i';E) = \sum_{n=1}^{\infty} \frac{\lambda_{nl}^{(i)}(E)}{1-\lambda_{nl}^{(i)}(E)} \varphi_{nl}^{(i)}(p_i;E) \varphi_{nl}^{(i)}(p_i';E) \quad (4)$$

($t_l^{(i)}$ is the partial scattering amplitude of particles j and k, $j \neq k \neq i$; in (2) and (4) the following numbering of particles is adopted: $1, 2$ are electrons, 3 is the proton). Here $\varphi_{nl}^{(i)}(p_i;E)$ is the momentum representation of the eigenfunctions of the radial Schrödinger equation with the potential $V_i(r_{jk})/\lambda_{nl}^{(i)}(E)$. The index n, numbering the terms in the expansion (4), may be interpreted as the principal quantum number.

The first approximation in the separable expansion of the pair amplitudes corresponds to $n = 1$, $l = 0$ (the $1s$-approximation). In this approximation, for singlet scattering we have a system of two integral equations

$$\chi_{10}^{(+)}(q) = \eta_{10}^{(2)}(q) + \int_0^\infty dq'^2 K_{10,10}^{12}(q;q') \chi_{10}^{(+)}(q') + 2 \int_0^\infty dq'^2 K_{10,10}^{13}(q;q') \chi_{10}^{(3)}(q'),$$

$$\chi_{10}^{(3)}(q) = \eta_{10}^{(3)}(q) + \int_0^\infty dq'^2 K_{10,10}^{31}(q;q')\chi_{10}^{(+)}(q'). \tag{5}$$

The inhomogeneous term $\eta_{10}^{(1)} = 0$ by virtue of the boundary conditions (3) (it is assumed that before scattering the bound state is formed by particles 2 and 3). The solution of system (5) presents no serious difficulties. The integral terms were written in the form of an integral sum. Truncating each sum at ~ 30 terms reduces (5) to a system of 60 linear algebraic equations. Its solution on the M-2 computer at the Institute of Theoretical and Experimental Physics takes less than a minute of machine time. In this way we obtained $\chi_{10}^{(+)}(0) = -1.22$, i.e., the singlet scattering length in the $1s$-approximation is $a_{1s}^{+} = 6.01$. Thus, already the first term of the separable expansion gave a very good result. The value a_{1s}^{+} agrees to hundredths with the presently accepted best value of the singlet scattering length $a^{+} = 5.961$, obtained from variational calculations ([5]).

For triplet scattering in the lowest $1s$-approximation we have one integral equation:

$$\chi_{10}^{(-)}(q) = -\eta_{10}^{(2)}(q) - \int_0^\infty dq'^2 K_{10,10}^{12}(q;q')\chi_{10}^{(-)}(q'). \tag{6}$$

The solution of equation (6) gives $\chi_{10}^{(-)}(0) = 0.632$; in this case the triplet scattering length is $a_{1s}^{-} = 3.12$. The best result for the triplet scattering length, obtained by the variational method, is $a^{-} = 1.768$ ([5]), i.e., it differs from ours by almost a factor of two.

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* In Ref. ([3]) additional conditions are imposed on the functions $\chi_{nl}^{(i)}$: for total spin of the two electrons $S = 0$,

$$\chi_{nl}^{(1)} = (-1)^l \chi_{nl}^{(2)}, \qquad \chi_{nl}^{(3)} = 0$$

for odd l; for $S = 1$,

$$\chi_{nl}^{(1)} = (-1)^{l+1} \chi_{nl}^{(2)}, \qquad \chi_{nl}^{(3)} = 0$$

for even l. These conditions are incompatible with system (2); their use seems to us superfluous and erroneous. (This should lead to an incorrect estimate of the higher approximations in Ref. ([3]).) The identity of the electrons is in fact manifested in the conditions (3); the Pauli principle is already contained in expression (1).

Thus, we see that the situation is different in triplet and singlet scattering. The physical reason for this difference apparently lies in the fact that the lowest $1s$-approximation in the triplet case does not contain the amplitude of electron-electron ($e-e$) scattering, whose magnitude can to a large extent determine the

final result. The contribution of the $e-e$ amplitude to triplet scattering arises from the next approximation in the separable expansion (4), which corresponds to taking into account terms with $n=2,\ l=0,1$ (the $2s$-, $2p$-approximation). In the $1s-2s-2p$ approximation, determining the function $\chi_{10}^{(-)}(q)$ leads to a system of 4 integral equations. At present we are unable to investigate its solution. This problem is not difficult, but it requires computers more modern than the M-20, which has a relatively small machine memory.

Note added in proof. After the manuscript had been sent to press, the authors learned from a notice in Phys. Rev. Lett., **22**, No. 23 (1969), in the section "Abstracts of articles to be publ. in P. R.," of the existence of an article by J. Chen, K. Chung, P. Kramer, "Faddeev equations for atomic problems. II," received by the editors of Phys. Rev. on 14 February 1969 and devoted, in particular, to the consideration of analogous questions.

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Note: Figure translations are in progress. See original paper for figures.