

Iterative solution of bound-state equations

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A method is proposed for solving bound-state equations in the momentum space, which are homogeneous Fredholm integral equations of the second kind. We rewrite such equations in the form of equivalent inhomogeneous Fredholm integral equations of the second kind with "weaker" kernels. Then the usual techniques for solving inhomogeneous integral equations can be used in the present case. A recently proposed method for an iterative Neumann series solution of inhomogeneous equations appears to be natural and very suitable for our purpose. The method is illustrated numerically in the case of the two nucleon bound state with the Yukawa and the Malfliet-Tjon potential and in the case of the s -wave three nucleon bound state in the Mitra-Amado model.

NUCLEAR STRUCTURE Bound state equations, equivalent inhomogeneous integrals equations, iterative solution, two-nucleon system with Yukawa-type potential, three-nucleon system in the Mitra-Amado model, wave function calculated in the momentum space.

I. INTRODUCTION

Calculation of the bound-state wave function in the coordinate space for a few-body system involves solving a single or a set of coupled second order differential equations. Numerical solution of such equations is not a simple task especially for potentials with a soft core.¹ On the other hand, in the momentum space after partial wave projection we have a single or a set of coupled homogeneous Lippmann-Schwinger-type integral equations with a smooth kernel² and the numerical solution of such equations appears to be simpler for certain problems of physical interest. The homogeneous integral equation has a Fredholm kernel³ and such an equation can be uniformly approximated by a matrix equation of finite rank, which can be solved by standard techniques. In the case of a realistic problem the dimension of the resulting matrix equation could be large and an eigenfunction problem involving a large matrix is a complicated numerical task.

Here we propose a simple method for solving the bound-state problem in the momentum space. We rewrite the bound-state homogeneous Fredholm integral equation in the form of an equivalent inhomogeneous Fredholm integral equation.³ The equivalence between the homogeneous and the inhomogeneous equations is discussed. The equivalent inhomogeneous equation has a "weaker" kernel and a recently proposed method^{4,5} for the iterative solution of the inhomogeneous equation appears to be attractive for our purpose. The method is illustrated numerically in the case of the two- and three-nucleon systems using the iterative Neumann series solution of the equivalent inhomogeneous equation. The s -wave two-nucleon problem we solve uses the Yukawa and the

Malfliet-Tjon potentials.^{5,6} The s -wave spin-doublet three-nucleon problem we solve uses the s -wave separable interaction with the Yamaguchi form factor.⁷ This model for the three nucleon bound-state problem was first studied by Mitra⁸ and is commonly known as the Mitra-Amado model.

In Sec. II we describe the present method for single-channel and multichannel problems. In Sec. III we present numerical results for the two- and three-nucleon system. Finally in Sec. IV we give a brief discussion and concluding remarks.

II. THE METHOD

A. Single channel problem

A single channel one variable partial-wave homogeneous Lippmann-Schwinger-type equation for the bound-state wave function ψ can be written as

$$\psi(p; E) = \frac{2}{\pi} G_0(p) \int dq q^2 V(p, q) \psi(q; E) \quad (2.1)$$

with $G_0(p) = (E - p^2)^{-1}$ in units $\hbar = 2\mu = 1$, where p, q are momentum variables and μ is the reduced mass. (Here E is negative and $|E|$ is the binding energy of the system.) Unless otherwise specified the integration limits in Eq. (2.1) and in the rest of the paper are from 0 to ∞ .

Now we use the techniques of Ref. 9 to rewrite Eq. (2.1) in the form of an equivalent inhomogeneous integral equation. It is obvious and well known that Eq. (2.1) does not determine the normalization of the unknown wave function $\psi(p; E)$. We normalize $\psi(p; E)$ such that

$$\frac{2}{\pi} \int \gamma(p) \psi(p; E) p^2 dp = 1, \quad (2.2)$$

where $\gamma(p)$ is an arbitrary function to be defined later. Using Eqs. (2.1) and (2.2) we have

$$\psi(p; E) = G_0(p) \left(V(p, k) + \frac{2}{\pi} \int dq q^2 [V(p, q) - V(p, k)\gamma(q)] \psi(q; E) \right), \quad (2.3)$$

where k is an arbitrary chosen point in the interval $(0, \infty)$. With the normalization given by Eq. (2.2) the solution $\psi(p; E)$ of Eq. (2.1) satisfies the equivalent inhomogeneous equation (2.3).

We must note that Eq. (2.1) has a solution for certain selected energies, namely, when $E = -B$, where B corresponds to the binding energy of the system; whereas Eq. (2.3), being an inhomogeneous equation, has a unique solution for all energies unless the homogeneous version of Eq. (2.3) has a solution. An interesting question to ask at this stage is that by solving Eq. (2.3) how can we calculate the binding energy B and the eigenfunction $\psi(p; E)$ of the system? By construction, all the solutions of Eq. (2.3), which also satisfy Eq. (2.2), are solutions of Eq. (2.1). So one should solve Eq. (2.3) for a particular E and check whether this solution also satisfies Eq. (2.2). If it does, then for this energy there is a bound state of the system and the solution of Eq. (2.3) gives the exact eigenfunction. Alternatively, if the energy eigenvalue for which Eq. (2.1) has a solution is given, then for this energy the solution of Eq. (2.3) gives the correct eigenfunction.

Equation (2.3), being an inhomogeneous Fredholm integral equation of the second kind, can be solved by standard methods as the Fredholm alternative is valid.³ From a glance at Eq. (2.3) we realize that a recently proposed method,^{4, 5, 10} for the iterative solution of such an equation is very suitable for our purpose. In fact, the kernel of Eq. (2.3) is very similar to the kernel of Eq. (1.2) of Ref. 10. Hence as in Ref. 10 we use^{10, 11}

$$\gamma(q) = \frac{\int \omega(p) dp V(p, k) V(p, q)}{\int \omega(p) dp V(p, k) V(p, k)} \quad (2.4)$$

and expect that such a γ will give a convergent iterative solution of Eq. (2.3). Such a choice of γ satisfies $\gamma(k) = 1$. Hence the kernel of Eq. (2.3) will have a zero for $q = k$ and is expected to be small for other values of q . As in Refs. 10 and 11 we use simple analytic forms for $\omega(p)$, e.g., $\omega(p) = p^n$, where n is a small positive or negative integer provided that the integrals in Eq. (2.4) remain finite for such a choice. Such a $\omega(p)$ suppresses or enhances parts of the integrals in Eq. (2.4) and hence generates a wide class of $\gamma(q)$. The only arbitrariness we now have is in the choice of the point k and the function $\omega(p)$. As in

Refs. 10 and 11 we shall see in our numerical studies that this arbitrariness can be turned to good advantage—we can vary k and $\omega(p)$ in order to obtain the best convergence of the Neumann series of Eq. (2.3).

B. Multichannel problems

The method of the last subsection can be easily extended to the case of multichannel problems. In explicit notation the multichannel generalization of Eq. (2.1) becomes⁵

$$\psi_\alpha(p_\alpha; E) = G_\alpha(p_\alpha) \sum_\beta \int dq_\beta q_\beta^2 V_{\alpha\beta}(p_\alpha, q_\beta) \psi_\beta(q_\beta; E), \quad (2.5)$$

where $G_\alpha(p_\alpha) = f_\alpha(p_\alpha)(E_\alpha - p_\alpha^2)^{-1}$, E_α is the energy for channel α in fm^{-2} , and $f_\alpha(p_\alpha)$ is some weight function. Now we normalize $\psi_\alpha(p_\alpha; E)$ such that, for $\alpha = \alpha_0$, $\psi_{\alpha_0}(p_{\alpha_0}; E)$ satisfies

$$\int \gamma_{\alpha_0}(p_{\alpha_0}) \psi_{\alpha_0}(p_{\alpha_0}; E) p_{\alpha_0}^2 dp_{\alpha_0} = 1, \quad (2.6)$$

where, as before γ_{α_0} is an arbitrary function to be defined later. Equations (2.5) and (2.6) yield

$$\begin{aligned} \psi_\alpha(p_\alpha; E) &= G_\alpha(p_\alpha) \left(V_{\alpha, \alpha_0}(p_\alpha, k_{\alpha_0}) \right. \\ &\quad \left. + \sum_\beta \int dq_\beta q_\beta^2 [V_{\alpha\beta}(p_\alpha, q_\beta) - V_{\alpha\beta}(p_\alpha, k_\beta) \right. \\ &\quad \left. \times \gamma_\beta(q_\beta) \delta_{\beta, \alpha_0}] \psi_\beta(q_\beta; E) \right), \end{aligned} \quad (2.7)$$

where k_{α_0} is an arbitrarily chosen point. With the normalization (2.6) the solution $\psi_\alpha(p_\alpha; E)$ of Eq. (2.5) satisfies the equivalent inhomogeneous equation (2.7).

The discussion after Eq. (2.3) of the last subsection is valid in the present case and without reiterating the discussion we mention some of the interesting points of the present case. The recipe is to solve Eq. (2.7) for a particular energy and verify if this solution also satisfies Eq. (2.6). If it does, then this energy corresponds to the energy of a bound state of the system and the solution of Eq. (2.7) gives the eigenfunction of the system. In this case we choose $\gamma_{\alpha_0}(p_{\alpha_0})$ as in Refs. 10 and 11:

$$\gamma_{\alpha_0}(q_{\alpha_0}) = \frac{\sum_\alpha \int \omega(p_\alpha) dp_\alpha V_{\alpha, \alpha_0}(p_\alpha, k_{\alpha_0}) V_{\alpha, \alpha_0}(p_\alpha, q_{\alpha_0})}{\sum_\alpha \int \omega(p_\alpha) dp_\alpha V_{\alpha, \alpha_0}(p_\alpha, k_{\alpha_0}) V_{\alpha, \alpha_0}(p_\alpha, k_{\alpha_0})}. \quad (2.8)$$

As before, in Eq. (2.8) we take $\omega(p) = p^n$, where n

is a small integer and n and k_{α_0} will be chosen after some experimentation in order to have the "best" convergence of the iterative Neumann series solution of Eq. (2.7).

III. NUMERICAL CALCULATION

In this section we test the method numerically for the two commonly studied few-nucleon systems. First we study the case of the model s -wave two-nucleon system interacting via the Yukawa and the Malfliet-Tjon potentials.⁶ The parameters for these potentials have appeared in Ref. 5 and we do not quote them here. Next we study the interesting case of the s -wave spin doublet three-nucleon system interacting via the pairwise s -wave potential—commonly known as the Mitra-Amado model.⁸ This is the homogeneous version of the Amado model⁸ we studied previously.^{10,11} The potential parameters for this case have appeared in Ref. 11, which we use in the present work.

We map the momentum space integrals in p from 0 to ∞ to integrals in x , on the range -1 to $+1$, by the transformation

$$p = c \frac{1+x}{1-x}, \quad (3.1)$$

and approximate the x integral from -1 to $+1$ by Gauss-Legendre quadrature points.

First we present numerical results for the two nucleon system. In this case we took c of Eq. (3.1) to be 5 fm^{-1} and we took 32 points to approximate the x integral between -1 to $+1$. We solve Eq. (2.3) for various E by iteration and find after some experimentation that the best convergence was obtained for $\omega(p) = p^2$ in both the cases with (a) $k = 0.7 \text{ fm}^{-1}$ in the case of the Yukawa potential; and with (b) $k = 0.6 \text{ fm}^{-1}$ in the case of the Malfliet-Tjon potential, for energies around the bound-state energy of the system. If the solution of Eq. (2.3) at a particular energy satisfies Eq. (2.2), then this energy corresponds to the bound state energy and the solution of Eq. (2.3) gives the energy eigenfunction. The energy eigenvalue so obtained is given by $E = -2.23992 \text{ MeV}$ for the Yukawa potential and is given by $E = -0.35003 \text{ MeV}$ for the Malfliet-Tjon potential. The iterative solution of Eq. (2.3) in these cases is shown graphically in Figs. 1(a) and 1(b). The wave functions after a small number of iterations (specially $N=0$) are not very good in these cases, but the final convergence is very good. In this connection we note that although the final converged result of Fig. 1 satisfies the normalization condition given by Eq. (2.2), the wave functions of Fig. 1 are not normalized in a particular way for small number of iterations. In order to do more justice to our

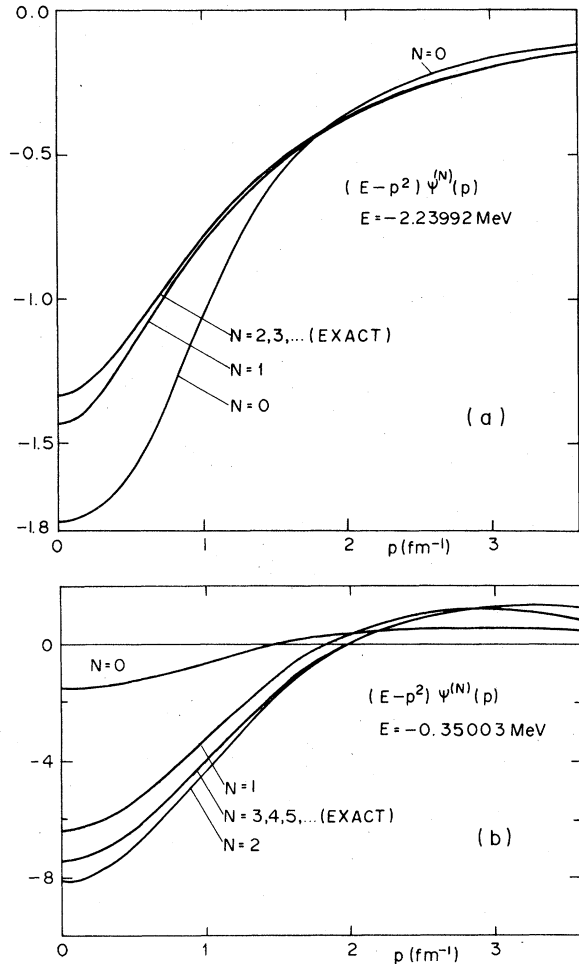


FIG. 1. The wave function $\psi^{(N)}(p; E)$ in the momentum space for various iterations N of Eq. (2.3) with (a) the Yukawa and (b) the Malfliet-Tjon potential. The quantities plotted are $(E - p^2)\psi^{(N)}(p; E)$. Note that $(E - p^2)\psi^{(0)}(p; E) = V(p, k)$.

iterative solutions we prefer to normalize them such that for every iteration N the normalized wave function $\bar{\psi}$ satisfies

$$\bar{\psi}^{(N)}(p; E) = \frac{\psi^{(N)}(p; E)}{\psi^{(N)}(0; E)}. \quad (3.2)$$

It should be noted that $\bar{\psi}(p; E)$ after such normalization no longer satisfies Eq. (2.3) but satisfies only Eq. (2.1). The iterative solutions for the wave functions after such normalization are shown in Tables I and II for the Yukawa and the Malfliet-Tjon potentials, respectively.

The normalization condition given by Eq. (2.2) is satisfied only with the converged wave function. The integrals in Eq. (2.2) calculated numerically using the solution of Eq. (2.3) after eight iterations, for the Yukawa and Malfliet-Tjon potentials, were 1.00000 and 1.00010, respectively.

TABLE I. The wave function $\bar{\psi}^{(N)}(p; E)$ for the Yukawa potential for various iterations N of Eq. (2.3) and normalized according to Eq. (3.2). The quantities in the last column labeled (*) have been calculated, as explained in the text, by evaluating the right hand side of Eq. (2.1) directly using the converged solution of Eq. (2.3).

$p \backslash N$	0	1	2	3	4	5, 6, . . .	(*)
0.00	1	1	1	1	1	1	1
0.05	0.955 05	0.953 64	0.953 91	0.953 97	0.953 98	0.953 98	0.953 98
0.10	0.841 23	0.836 35	0.837 29	0.837 49	0.837 51	0.837 52	0.837 52
0.20	0.567 39	0.554 87	0.557 31	0.555 83	0.557 89	0.557 89	0.557 89
0.40	0.238 57	0.221 49	0.224 98	0.225 72	0.225 80	0.225 81	0.225 81
0.60	0.112 57	0.100 03	0.102 89	0.103 47	0.103 54	0.103 54	0.103 54
0.80	0.057 71	0.051 30	0.053 15	0.053 52	0.053 56	0.053 56	0.053 56
1.00	0.031 02	0.028 95	0.030 02	0.030 22	0.030 24	0.030 24	0.030 24
2.00	0.002 76	0.003 52	0.003 69	0.003 71	0.003 71	0.003 71	0.003 71
3.00	0.000 57	0.000 83	0.000 89	0.000 90	0.000 90	0.000 90	0.000 90

The agreement between the numerical value of the integral in Eq. (2.2) and unity gives a good measure of the precision of the method. This was easily verified by substituting the converged solution of Eq. (2.3) in the integral in Eq. (2.1), by evaluating this integral numerically and by comparing the result with the solution of Eq. (2.3). In Tables I and II, in the last column we show $\bar{\psi}(p; E)$ so calculated by using Eq. (2.1) and normalized according to (3.2), and as expected it agrees very well with the converged result of Eq. (2.3). When the solution $\psi(p; E)$ of Eq. (2.3) satisfied Eq. (2.2) accurately it also satisfied Eq. (2.1) accurately. It was verified that the percentage of numerical error in the solution $\psi(p; E)$ of Eq. (2.3) is less than the percentage of error in the numerical evaluation of the integral in Eq. (2.2) using the solution of Eq. (2.3).

In the case of the s -wave spin doublet three nucleon Mitra-Amado model⁸ there are two channels defined by $\alpha = 0, 1$.¹¹ In order to be consistent with the definitions given in Ref. 11 we had to re-define here the function $G_\alpha(p_\alpha)$ that appears in

Sec. II B. In Eqs. (2.5)–(2.7) we define

$$G_\alpha(p) = \frac{-3}{2\pi} F_\alpha(s - \frac{3}{4}p^2), \quad (3.3)$$

where F_α is defined by Eq. (3.15) of Ref. 11. All other parameters and variables are defined in Ref. 11, except that here we use the variable V instead of the variable Z of Ref. 11. In this case we take $\alpha_0 = 0$, where the channels 0 and 1 have the same meaning as in Ref. 11. In Eq. (3.1) we use $c = 0.1 \text{ fm}^{-1}$ and 32 points were used to represent the integral in x as a discrete sum. We solve (2.7) by iteration and the best convergence was obtained for $\omega(p) = p^3$ and $k_0 = 0.7 \text{ fm}^{-1}$ in Eqs. (2.6)–(2.8). The energy eigenvalue in this case was given by $E = -11.0047 \text{ MeV}$ and at this energy the solution of Eq. (2.7), after eight iterations, was used to calculate the integral in Eq. (2.6), which yielded the value 1.000 000. As before, the close agreement between this value and unity gives a good idea of the precision of the method. In Table III we show the iterative solution $\psi_0(p; E)$ of Eq. (2.7), normalized as in Eq. (3.2), for E

TABLE II. Same as in Table I for the Malfliet-Tjon potential.

$p \backslash N$	0	1	2	3	4, 5, . . .	(*)
0.00	1	1	1	1	1	1
0.05	0.770 02	0.770 24	0.770 29	0.770 29	0.770 29	0.770 29
0.10	0.454 23	0.454 75	0.454 87	0.454 88	0.454 88	0.454 88
0.20	0.168 98	0.169 77	0.169 95	0.169 97	0.169 97	0.169 97
0.40	0.044 25	0.045 14	0.045 35	0.045 37	0.045 37	0.045 37
0.60	0.017 20	0.018 07	0.018 29	0.018 33	0.018 32	0.018 32
0.80	0.007 67	0.008 49	0.008 71	0.008 75	0.008 74	0.008 74
1.00	0.003 47	0.004 23	0.004 44	0.004 48	0.004 47	0.004 47
2.00	-0.000 51	-0.000 11	-0.000 01	-0.000 01	-0.000 01	-0.000 01
3.00	-0.000 39	-0.000 19	-0.000 16	-0.000 17	-0.000 17	-0.000 17

TABLE III. The wave function $\bar{\psi}^{(N)}(p; E)$ for the s -wave Mitra-Amado model for various iterations N of Eq. (2.7) and normalized according to Eq. (3.2). The quantities in the last column labeled (*), as explained in the text have been calculated by evaluating the right hand side of Eq. (2.5) directly using the converged solution of Eq. (2.7).

$p \backslash N$	0	1	2	4	6	7, 8...	(*)
0.00	1	1	1	1	1	1	1
0.05	0.991 70	0.990 74	0.990 46	0.990 46	0.990 47	0.990 47	0.990 47
0.10	0.967 55	0.963 87	0.962 81	0.962 80	0.962 83	0.962 83	0.962 83
0.20	0.880 71	0.868 39	0.864 90	0.864 89	0.865 00	0.865 01	0.865 01
0.40	0.638 05	0.611 95	0.604 88	0.605 24	0.605 51	0.605 52	0.605 52
0.60	0.417 38	0.393 13	0.387 19	0.388 30	0.388 60	0.388 62	0.388 62
0.80	0.261 21	0.246 11	0.243 25	0.244 94	0.245 22	0.245 22	0.245 22
1.00	0.161 42	0.154 44	0.154 07	0.155 99	0.156 21	0.156 21	0.156 21
2.00	0.017 64	0.019 44	0.020 72	0.021 64	0.021 70	0.021 70	0.021 70
3.00	0.002 99	0.003 75	0.004 21	0.004 51	0.004 52	0.004 52	0.004 52
4.00	0.000 71	0.000 98	0.001 14	0.001 24	0.001 25	0.001 25	0.001 25

= -11.0047 MeV. In the last column of Table III we exhibit $\psi_0(p; E)$ calculated by using Eq. (2.5), which uses in its integrand the converged iterative solution of $\psi_0(p; E)$ and $\psi_1(p; E)$. The entries in this last column are also normalized as in Eq. (3.2).

IV. DISCUSSION

Here we propose a method for solving the partial wave momentum space Schrödinger equation for the bound state of few nucleon systems. Such equations have the form of homogeneous Fredholm integral equations and are written in the form of equivalent inhomogeneous Fredholm integral equations which are solved by iteration. The present method is expected to be simple and accurate numerically. This is because the only numerical work needed in this method is the evaluation of a small number of integrals and there is no loss of accuracy as in complicated numerical processes

such as diagonalization and/or calculation of the determinant of large matrices as required by other methods for solving such equations.

Even with the ideal choice of γ and k the equivalent inhomogeneous equation may not have a rapidly convergent iterative Neumann series solution if the kernel of Eq. (2.3) is not weak. But in such cases following Refs. 4 and 10 we can introduce an auxiliary equation with a reduced kernel, which has a rapidly convergent iterative solution. Then the solution of the equivalent inhomogeneous equation can be expressed in terms of some simple integrals involving the solution of the auxiliary equation.

The final result—Tables I–III and Fig. 1—demonstrate that the present method is a simple, accurate, and efficient alternative for solving the bound state problem for the few nucleon system.

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¹See, for example, A. Laverne and C. Gignoux, Nucl. Phys. A203, 597 (1973); G. L. Payne, J. L. Friar, B. F. Gibson, and I. R. Afnan, Phys. Rev. C 22, 823 (1980); T. Sasakawa and T. Sawada, *ibid.* 19, 2035 (1979).

²See, for example, E. P. Harper, Y. E. Kim, and A. Tubis, Phys. Rev. C 6, 1601 (1972); W. M. Kloet and J. A. Tjon, Nucl. Phys. A176, 481 (1971); I. R. Afnan and N. D. Birrell, Phys. Rev. C 16, 823 (1977).

³See, for example, E. T. Whittaker and G. N. Watson, *A Course of Modern Analysis*, fourth ed. (Cambridge University Press, Cambridge, 1927), Chapter XI; P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill, New York, 1953), Chap. 8.

⁴S. K. Adhikari, J. Comp. Phys. (to be published).

⁵L. Tomio and S. K. Adhikari, Phys. Rev. C 22, 2359 (1980); S. K. Adhikari, *ibid.* 19, 1729 (1979); L. Tomio and S. K. Adhikari, *ibid.* 22, 28 (1980).

⁶R. A. Malfliet and J. A. Tjon, Nucl. Phys. A127, 161 (1969).

⁷Y. Yamaguchi, Phys. Rev. 95, 1628 (1954).

⁸A. N. Mitra, Nucl. Phys. 32, 529 (1962); R. D. Amado, Phys. Rev. 132, 485 (1963).

⁹S. K. Adhikari (unpublished).

¹⁰L. Tomio and S. K. Adhikari, Phys. Rev. C 24, 43 (1981).

¹¹See the first article of Ref. 5.