Upper and Lower Bound of the Eigenvalue of a Three-Body System*

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A variational calculation is performed to determine the upper and lower bound of the eigenvalue of the ground state of a three-body system with two types of two-body, central potential without hard core. The trial wave function used is a function which is a product of the solution of the two-nucleon Schrödinger equation up to a certain internucleon separation, which goes over into a variation function for larger distances. The calculation is done by a Monte Carlo method. The results show that with this type of trial wave function, the upper and lower bound are rather close to each other, with the difference between the values of the two bounds equal to only about 3% of the magnitude of the upper bound.

I. INTRODUCTION

WHEN a two-body potential with a hard core is used in a variational calculation to determine the binding energy of a few-body system, it is necessary to choose a trial wave function which can allow for a faithful reproduction of the behavior of the exact wave function immediately outside the region of the hard core, where the attractive potential has a large depth. If the trial wave function fails to meet this requirement, the upper bound obtained will, in general, be rather far away from the eigenvalue. To deal with calculations of this kind in which a hard-core potential is involved, Austern and Iano[1] have recently proposed a type of trial wave function which focuses particular attention on the region of strong attractive interaction. In this type, the trial wave function is chosen as a product of the solution of the two-body Schrödinger equation up to a certain internucleon separation which goes over into a variational function for larger distances. To test the usefulness of this type of trial function, calculations have been made to determine the binding energy of a two-body system with a square-well potential containing a hard core[1] and to find the energy of the $^{31}S_0$ state in Li^6.[2] In the former case, an upper bound of -3.92 MeV is obtained, which is to be compared with the eigenvalue of -4.13 MeV. The fact that there is still a comparatively large difference of 0.21 MeV between the upper bound and the eigenvalue arises as a consequence of the choice of a square well as the shape of the two-body potential. The discontinuity in this potential necessitates choosing the separation distance in the trial wave function to be at the edge of the square-well potential,[3] which was purposely not done by Austern and Iano. However, the advantage of this type of trial wave function was still clearly demonstrated over many other types of trial functions.[1] In the case of Li^6, it was also found that the determination of the energy of the $^{31}S_0$ state can be made more reliable with this type of trial wave function. However, due to some approximations made in their calculation, it was not possible to discuss how close the upper bound is to the energy of this state. In our opinion, therefore, these two examples show quite impressively the promise of this type of wave function in variational calculations on few-body problems, but do not demonstrate the degree of accuracy which one can hope to achieve with this wave function.

In this investigation, we shall calculate with this type of wave function both the upper and the lower bound of the energy eigenvalue of a three-body system. The two-body potentials used will not contain a hard core; they will be those which have been utilized in accurate calculations performed by other investigators. From the values of these two bounds, we will gain some information about how good this trial wave function is. It is true, of course, that from this study, no definitive statement can be made concerning the accuracy of this type of trial function in the case where a hard-core two-body potential is involved. However, if the two bounds should turn out to be close to each other, then this calculation would at least serve to give the indication that further calculation with hard-core potential using this trial function may also yield upper bound which is fairly close to the eigenvalue.

The method of calculation is discussed in the next section. In Sec. III, the numerical results will be presented and in Sec. IV, a discussion of the results will be made.

II. METHOD OF CALCULATION

The upper bound will be computed by the usual Rayleigh-Ritz method, i.e.,

$$E_0 \leqslant E_u = \langle H \rangle, \tag{1}$$

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[1] N. Austern and P. Iano, Nucl. Phys. **18**, 672 (1960).

[2] P. H. Wackman and N. Austern, Nucl. Phys. **30**, 529 (1962).

[3] E. W. Schmid, Y. C. Tang, and R. C. Herndon, Nucl. Phys. **42**, 247 (1963).

where E_0 is the lowest eigenvalue of the Hamiltonian. For the lower bound, we adopt a method of Temple[5] which gives

$$E_0 \geqslant E_L = \langle H \rangle - (\langle H^2 \rangle - \langle H \rangle^2)/(E_1 - \langle H \rangle), \quad (2)$$

with E_1 being the exact energy of the first excited state having the same symmetry property as the ground state. The choice of the two-body potentials used in this investigation will insure that E_1 denotes the energy of the configuration in which two particles form a bound state and the third particle is far away. Thus, E_1 can be obtained quite easily by a numerical solution of the two-body Schrödinger equation.

It might be appropriate to mention here that if a trial wave function is capable of reproducing faithfully the behavior of the exact wave function in the region of small internucleon separation and has enough flexibility at larger distances, the computation of the lower bound can be very fruitful. In a previous calculation,[4] we have demonstrated this point by a calculation on a two-body system using a potential of the Yukawa shape and a Hulthèn-type trial wave function. For an eigenvalue of -2.3071 MeV, the upper and lower bound obtained were -2.3054 and -2.3640 MeV, respectively. Thus, in this particular instance, the gap between the two bounds is only 3% of the eigenvalue, which shows clearly the usefulness of the lower-bound method.

For convenience, we shall consider our three-body system as a fictitious triton. Since, in this investigation, the trial wave function will be assumed to contain only the configuration in which the two neutrons are in a space-symmetric state, the spatial part can be written as

$$\psi = f(r_{12})g(r_{13})g(r_{23}), \quad (3)$$

in which 1, 2 denote the neutrons and 3 denotes the proton. For the function $f(r)$, we use

$$f(r) = U_f(r)/r, \qquad (r < d_f)$$
$$= \frac{A_f[\exp(-\alpha_f r) + B_f \exp(-\beta_f r)]}{r^{1/2}} \qquad (r > d_f), \quad (4)$$

where $U_f(r)$ is a solution of the equation

$$-\frac{\hbar^2}{m}\frac{d^2}{dr^2}U_f(r) + [V_f(r) - e_f]U_f(r) = 0, \quad (5)$$

with $V_f(r)$ being the effective potential between the neutron pair. The constants A_f and B_f in Eq. (4) are adjusted such that the function $f(r)$ and its first derivative are continuous at the separation distance d_f. There are a total number of four variational parameters in this function, namely, e_f, d_f, α_f, and β_f. The function $g(r)$ is defined in a similar fashion, except that the potential function in Eq. (5) is replaced by the effective potential $V_g(r)$ between a neutron-proton pair. The variational parameters in this latter function are e_g, d_g, α_g, and β_g.

If the two-body potential used is spin-independent, the functions $f(r)$ and $g(r)$ are identical. In this case, the total number of variational parameters will then be only four, i.e., e, d, α, and β.

The factor $r^{1/2}$ in the functions $f(r)$ and $g(r)$ is chosen such that the asymptotic behavior is given correctly. For instance, when the proton is far away from the two neutrons, the wave function ψ takes on the asymptotic form

$$\psi \sim f(r_{12})\exp(-2\alpha_g R)/R, \quad (6)$$

where R is the distance from the proton to the center of mass of the two neutrons. The parameter α_g is thus related to the separation energy of the proton. If we have some idea about the magnitude of this separation energy, a fairly good guess for the value of α_g to start the variational process can then be obtained. This is useful in a variational calculation, since if one can start with a set of values for the parameters which are close to the optimum values, the time of computation can be greatly reduced.

The starting point for the search of the optimum values of d_f, d_g, e_f, and e_g can also be fixed easily. It has been pointed out by Austern and Iano[1] that the upper bound is rather insensitive to these parameters. In our actual calculation, we have found that this is indeed so. Both the upper and the lower bound are especially insensitive to the variation of d_f and d_g. In fact, in some of the cases considered in this investigation, we have merely fixed them at a reasonable value without further variation. For e_f and e_g, our experience indicates that they can be set as zero initially. After the best values for α_f, α_g, β_f, and β_g are found, e_f and e_g are then varied to improve the value of the two bounds. In this manner, we can usually get the best possible values of the upper and lower bound obtainable with the type of trial wave function used in this investigation.

All the integrals which arise from the computation of the expectation value of the Hamiltonian and of the square of the Hamiltonian are done by a Monte Carlo method. As this method has already been discussed in detail previously,[4,6] we shall not discuss it further here.

The numerical calculation was carried out on an IBM-7094 computer. To insure a high degree of accuracy, double-precision arithmetic has been used in the computation whenever it was felt necessary.

III. NUMERICAL CALCULATIONS

Two types of central potential without hard core have been considered. These were the potentials used in the calculations of Rarita and Present[7] and of Baker *et al.*[8] We choose these potentials in this investigation since we

[4] E. W. Schmid, Y. C. Tang, and R. C. Herndon, Nucl. Phys. **42**, 95 (1963).
[5] G. Temple, Proc. Roy. Soc. (London) **119**, 276 (1928).
[6] E. W. Schmid, Nucl. Phys. **32**, 82 (1962).
[7] W. Rarita and R. D. Present, Phys. Rev. **51**, 788 (1937).
[8] G. A. Baker, Jr., J. L. Gammel, B. J. Hill, and J. G. Wills, Phys. Rev. **125**, 1754 (1962).

feel that the results obtained by these authors are quite accurate and hence, useful for purpose of comparison with the upper and lower bound obtained in this calculation.

A. Calculation with an Exponential Potential

The two-body potential used here is a potential with purely Majorana space-exchange character. It has

$$V_t(r)=-V_0\exp(-\kappa r),$$
$$V_s(r)=0.57V_t(r), \tag{7}$$

with

$$V_0=123.56\text{ MeV},\quad \kappa=1.156\text{ F}^{-1},$$

in the triplet-even and singlet-even state, respectively. This potential was used by Rarita and Present in a study of the two-, three-, and four-body problems.[7,9]

To test the accuracy of the Monte Carlo method, we have first computed with the potential given by Eq. (7) and a trial wave function which has a spatial part of the form

$$\psi=\exp[-\gamma(r_{12}+r_{13}+r_{23})]. \tag{8}$$

With this wave function, the expectation value of the Hamiltonian can be calculated analytically and the result is -7.470 MeV with $\gamma=0.39\text{ F}^{-1}$. With our Monte Carlo method, we get $E_u=-7.47\pm0.11$ MeV with 40 000 estimates. The amount of computing time needed on the IBM 7094 computer was 15 min.

For a two-body potential with spin dependence, the wave function for the triton has the form

$$\Psi=\psi_s\chi_a+\psi_a\chi_s, \tag{9}$$

where ψ_s and ψ_a are spatial wave functions which are symmetrical and antisymmetrical in the space coordinates of the two neutrons, respectively. The functions χ_a and χ_s are spin functions, with χ_a antisymmetrical and χ_s symmetrical in the spin coordinates of the two neutrons. Since the main purpose of this investigation is to examine how appropriate our trial wave function described by Eqs. (3)–(5) is as ψ_s, we shall ignore the part $\psi_a\chi_s$. Due to this simplification, our upper bound will be at least about 0.22 MeV different from the exact eigenvalue, as was found by Rarita and Present.[7]

The fact that we ignore the part $\psi_a\chi_s$ in Eq. (9) makes it necessary to compute the lower bound with effective potentials $V_f(r)$ of the neutron-neutron pair and $V_g(r)$ of the neutron-proton pair instead of the two-body potential given by Eq. (7). This is so, since otherwise, the gap between the two bounds would arise mainly as a consequence of our omission of the part $\psi_a\chi_s$ rather than from the inaccuracy of our trial wave function as against the best possible form of ψ_s. These effective potentials will also have a Majorana character and be of the form

$$V_f(r)=V_s(r),$$
$$V_g(r)=\tfrac{1}{4}V_s(r)+\tfrac{3}{4}V_t(r), \tag{10}$$

in the even orbital-angular-momentum states.

The search for optimum values in the 8-parameter space is done with 4000 estimates. After the search is over, more estimates are then taken to achieve the desired degree of statistical accuracy for both the upper and the lower bound. In total, the amount of computing time spent is about 3 h on the IBM 7094 computer.

With 35 000 estimates, we obtain

$$E_u=-7.81\pm0.07\text{ MeV},$$
$$E_L=-8.31\pm0.16\text{ MeV}, \tag{11}$$

with the uncertainty representing the standard deviation calculated by our Monte Carlo method. In the calculation of E_L, a value of E_1 equal to -1.06 MeV determined by solving the two-body Schrödinger equation with an effective potential $V_g(r)$ is used.

The optimum values of the parameters are $\alpha_f=0.23$ F^{-1}, $\beta_f=1.35$ F^{-1}, $d_f=1.2$ F, $e_f=4.0$ MeV, $\alpha_g=0.27$ F^{-1}, $\beta_g=1.65$ F^{-1}, $d_g=1.2$ F, $e_g=0$ for the upper bound and $\alpha_f=0.24$ F^{-1}, $\beta_f=1.30$ F^{-1}, $d_f=1.2$ F, $e_f=4.0$ MeV, $\alpha_g=0.26$ F^{-1}, $\beta_g=1.65$ F^{-1}, $d_g=1.2$ F, $e_g=-4.0$ MeV for the lower bound. As is expected, both the upper bound and the lower bound are insensitive to the parameters d_f and d_g. In fact, any value between 1.0 and 1.5 F seems to be appropriate.

The gap between the two bounds is only 0.5 MeV in this case. Since we know from our previous study on the deuteron[4] and from the calculation on the helium atom[10] that the eigenvalue is usually much closer to the upper bound than to the lower bound,[11] we are inclined to believe that the eigenvalue is probably not more than 0.05 MeV away from the upper bound. This shows that the trial wave function used here is a good approximation to the exact eigenfunction, which is also manifested by the fact that the optimum parameters for the upper bound are very nearly the same as those for the lower bound.

Rarita and Present[7] have examined the three-body problem using a Hylleraas-type variational function with a large number of parameters. The result they obtained with $\psi_s\chi_a$ part alone of Eq. (9) was -7.79 MeV for the upper bound, which is in very good agreement with our value given in Eq. (11).

We have also calculated with a two-body potential which is the same in the even state as that described by Eq. (7), but has no space-exchange dependence. With this potential, E_u is found to be -7.89 MeV, which is only 0.08 MeV more than that obtained with a Majorana-type force. This shows that the exact nature of the two-body potential in the odd orbital-angular-

[9] Rarita and Present (Ref. 7) used $\hbar^2/m=41.12$ MeV$-$F^2 in their calculation, while we use $\hbar^2/m=41.47$ MeV$-$F^2. However, all their results quoted here have been adjusted for this difference.

[10] T. Kinoshita, Phys. Rev. **115**, 366 (1959); **105**, 1490 (1957).

[11] G. L. Caldow and C. A. Coulson, Proc. Cambridge Phil. Soc. **57**, 341 (1961).

momentum state is not too important as far as its influence on the binding energy of the triton is concerned, which is of course to be expected from physical grounds.

Also, we have examined this problem with a trial wave function which is totally space symmetric, i.e., $f(r)=g(r)$. The purpose is to see how much worse the upper bound will be if such a simplified trial function is used. For the same reason as explained in a previous paragraph, the lower bound will again be calculated with effective potentials which have the form

$$V_f(r)=V_g(r)=\tfrac{1}{2}V_t(r)+\tfrac{1}{2}V_s(r), \tag{12}$$

in this case. The results we get with 40 000 estimates are

$$E_u=-7.65\pm0.05 \text{ MeV},$$
$$E_L=-7.84\pm0.11 \text{ MeV}. \tag{13}$$

Here, E_L is calculated with $E_1=-0.35$ MeV obtained with the effective potential $V_g(r)$. The optimum parameters are $\alpha=0.26$ F^{-1}, $\beta=1.60$ F^{-1}, $d=1.2$ F, $e=0$ for the upper bound and $\alpha=0.25$ F^{-1}, $\beta=1.60$ F^{-1}, $d=1.2$ F, $e=-1.0$ MeV for the lower bound. The closeness between the two bounds indicates that not much further improvement in the upper bound can be expected as a result of improving the function $f(r)$. If one wishes to obtain a value for the upper bound closer to the eigenvalue of the triton, then one should rather include the $\psi_a\chi_s$ part of Eq. (9) and make the function $f(r)$ not identical to $g(r)$.

From Eqs. (11) and (13), we see that the improvement in E_u, by using a function which is not totally space symmetric, is only 0.16 MeV. Thus, in a calculation where an improvement of this magnitude is not considered as important, one should certainly use a totally space-symmetric trial wave function, since the amount of computing time saved by reducing the number of variational parameters from eight to four will usually be substantial.

B. Calculation with a Gaussian Potential

The two-body potential used by Baker *et al.*[8] will be considered next. It has the form

$$V_t(r)=V_s(r)=-51.5\exp[-(r/b)^2]\text{MeV}, \tag{14}$$

with $b=1.60$ F. The interaction in the odd states does not need to be specified, since the lack of spin dependence insures the eigenfunction to be totally space symmetric.

We have also tested the Monte Carlo method with this two-body potential and a trial wave function which has a spatial part

$$\psi=\exp[-\lambda(r_{12}^2+r_{13}^2+r_{23}^2)]. \tag{15}$$

The upper bound can be calculated analytically in this case; it is -6.907 MeV with $\lambda=0.10$ F^{-2}. With the Monte Carlo method, we obtain $E_u=-6.89\pm0.06$ MeV after 60 000 estimates. The closeness of these two values again indicates that our Monte Carlo method yields accurate results.

Since with a spin-independent potential there are only four parameters in the trial wave function, the search for optimum values of the parameters can be done with a comparatively small amount of computing time. The results for the two bounds with 80 000 estimates are

$$E_u=-9.74\pm0.05 \text{ MeV},$$
$$E_L=-10.04\pm0.07 \text{ MeV}. \tag{16}$$

The value of E_1 in this case is -0.40 MeV.

The values of the optimum parameters are $\alpha=0.288$ F^{-1}, $\beta=5.15$ F^{-1}, $d=1.5$ F, $e=-2.0$ MeV at the upper bound and $\alpha=0.292$ F^{-1}, $\beta=2.55$ F^{-1}, $d=1.8$ F, $e=-0.6$ MeV at the lower bound. Although the values of β at the two bounds seem to be quite different, the wave functions do not differ by more than 2% at all values of internucleon distances which are of interest.

The gap in this case is 0.30 MeV, which is only about 3% of the value of the upper bound. This indicates again that the type of trial wave function described by Eqs. (3)–(5) is capable of yielding an upper bound very close to the eigenvalue. In this particular example, we think that the difference between the upper bound and the eigenvalue is in all likelihood less than 0.05 MeV.

It might also be interesting to estimate the accuracy of our trial function directly. For this purpose, let us write

$$\psi=(1-\epsilon^2)^{1/2}\psi_0+\epsilon\psi', \tag{17}$$

where

$$\langle\psi',\psi_0\rangle=0,$$
$$\langle\psi',\psi'\rangle=1, \tag{18}$$

and ψ_0 represents the normalized ground-state eigenfunction. The quantity ϵ is thus a parameter to measure the deviation of ψ from ψ_0. It is quite easy to show that[10]

$$\epsilon^2\leqslant(E_u-E_L)/(E_1-E_L). \tag{19}$$

With optimum parameters of the lower bound, E_u and E_L are -9.71 MeV and -10.04 MeV, respectively. Using these values, we get

$$\epsilon^2\lesssim0.04, \tag{20}$$

which in turn gives

$$\langle\psi,\psi_0\rangle\gtrsim0.98. \tag{21}$$

This shows that the trial function ψ is a good representation of the eigenfunction ψ_0 in this particular case.

With the same two-body potential but a different method of calculation, Baker *et al.*[8] obtained a value of -9.42 MeV for the energy of the three-body system,

while Kalos[12] obtained a value of −9.47 MeV. In comparing with our value of the upper bound, there is a difference of about 0.3 MeV.[13] Normally, a difference of this magnitude will not be considered as substantial, but since we consider the methods of both Baker *et al.* and Kalos as quite accurate, the fact that such a difference exists is somewhat astonishing. It is possible that the numerical accuracy of the result of Baker *et al.* may be impaired to a certain degree by their use of a rather large mesh spacing. In their numerical calculation, they used a mesh spacing of about 0.1 F, while we use a much smaller spacing of 0.005 F. In our code, such a small spacing is admissible, since double-precision arithmetic is employed whenever necessary to avoid error by truncation.

[12] M. H. Kalos, Phys. Rev. **128**, 1791 (1962).

[13] It is interesting to point out that already for a simpler trial wave function

$$\psi = \prod_{i<j=1}^{3} [\exp(-\alpha r_{ij}^2) + C\exp(-\beta r_{ij}^2)]$$

with three variational parameters, the upper bound is −9.63 ±0.04 MeV with 50 000 estimates.

IV. CONCLUSION

This investigation shows that the type of trial wave function used here is capable of yielding very accurate results. For both types of two-body potential considered, the gap between the upper and the lower bound is so small as to allow us to make a good estimate of the eigenvalue. Also, it is quite easy to employ this wave function in a numerical calculation. Although it may sometimes contain as many as eight parameters, at least four of them, namely, the separation distances d and the energy parameters e, can be assigned good starting values and need very little subsequent variation.

At present, we are using this type of trial wave function to investigate the binding energies of the alpha particle, the hypernuclei and the helium molecules. From the closeness of the upper and lower bound found in this calculation, we believe that reliable estimates of the binding energies will be obtained in all these cases.

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Mössbauer Effect in Tm^{169} and Total Internal Conversion of the 8.42-keV Transition*

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The absolute yield of the Mössbauer absorption of the 8.42-keV transition in Tm^{169} was determined for a thulium oxide and a thulium metal absorber. The 8.42-keV gamma ray was resolved from the L x rays of erbium by means of a flat lithium fluoride crystal diffraction spectrometer. From the observed Mössbauer absorption effect the total conversion coefficient $\alpha_{tot}=325\pm35$ and the magnetic transition rate of $B(M1, \frac{3}{2}\rightarrow\frac{1}{2})=5.1\times10^{-2}$ $(e\hbar/2Mc)^2$ was derived.

INTRODUCTION

THE total cross section for nuclear resonance scattering and, in particular, for Mössbauer scattering or absorption depends directly on the internal conversion coefficient of the gamma transition involved. It is important to have a knowledge of this coefficient if the aim of an experiment is to determine the Debye-Waller factors or to find the optimum conditions for a Mössbauer experiment. Conversely, the conversion coefficient can be deduced from a Mössbauer experiment if all the other conditions are known.

The present work deals with the determination of the conversion coefficient from studies of the Mössbauer effect in Tm^{169}. The 8.42-keV transition from the $\frac{3}{2}$ state to the $\frac{1}{2}$ ground state has been employed in several Mössbauer experiments.[1] This transition has predominantly magnetic-dipole character, and the state from which it originates is well understood[2] from the point of view of nuclear structure being a member of a rotational band. Its energy, however, is so low that a theoretical conversion coefficient can only be estimated from extreme extrapolations of Rose's[3] tables. Such an estimate is probably good to a factor of 2 only.

There is, however, an indirect way of estimating the value of the conversion coefficient. The lifetime of the

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[1] M. Kalvius, W. Wiedemann, R. Koch, P. Kienle, and H. Eicher, Z. Physik **170**, 267 (1962); M. Kalvius, P. Kienle, H. Eicher, and W. Wiedemann, *ibid.* **172**, 231 (1963); R. G. Barnes, E. Kankeleit, R. L. Mössbauer, and J. M. Poindexter, Phys. Rev. Letters **11**, 253 (1963); R. L. Cohen, Phys. Letters **5**, 177 (1963).

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[3] M. E. Rose, *Internal Conversion Coefficients* (North-Holland Publishing Company, Amsterdam, 1958).