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TRITON BINDING ENERGY CALCULATIONS IN A HARMONIC OSCILLATOR BASIS*

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Abstract

The triton binding energy is calculated in a harmonic oscillator basis using a single term separable potential and the Reid soft core potential.

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I. Introduction

Calculations of the binding energy of the triton with local nucleon-nucleon potentials are usually made with the aid of the variational principle. A trial wave function is selected having a form which is hoped to exploit all of the important features of the two-body potential under investigation, and its parameters are adjusted to minimize the energy of the three-body system. The value of variational calculations is limited only by the degree of insight used in the selection of the trial wave function, and, although this insight has been developed to a high degree for some potentials, it is appealing to generate the trial wave function in a completely systematic manner. The upper limits on the triton binding energy calculated with realistic potentials are often of little practical value. (For example, the most recent calculation with the Hamada-Johnston potential[1] yields an upper limit of +60 MeV which is far greater than the lower limit of 6.7 MeV.) A more systematic prescription for the construction of a trial wave function might be expected to provide some additional information regarding the convergence of the triton binding energy.

Our goal is thus to define a complete set of states for the three nucleon system and to construct and diagonalize the Hamiltonian matrix in a truncated basis of these states. Moshinsky, et al.[2] have shown that it is a relatively simple matter to generate such a complete set of states in a manner which is particularly convenient for numerical calculations. What we shall demonstrate in this paper is that a meaningful estimate of the triton binding energy can be obtained for realistic potentials with a practical number of states.

II. Construction of Three-Body States

We shall describe the triton bound state in terms of totally antisymmetric states of definite orbital angular momentum L, spin S, orbital permutation symmetry

[λ], total angular momentum J = 1/2, and isospin T = 1/2. The classification of three-body states according to their orbital permutation symmetry is useful since the triton wave function is expected to be composed primarily of [3]S and [21]D states,[3] and it may be desirable to exclude states having other symmetries from a calculation. As is usual, the most convenient coordinate system to use for the three-body calculation may be written in terms of the single particle coordinates as

$$\dot{\underset{\sim}{x}}_1 = \frac{1}{\sqrt{2}} (\underset{\sim}{x}_1 - \underset{\sim}{x}_2)$$

$$\dot{\underset{\sim}{x}}_2 = \frac{1}{\sqrt{6}} (\underset{\sim}{x}_1 + \underset{\sim}{x}_2 - 2\underset{\sim}{x}_3)$$

$$\dot{\underset{\sim}{x}}_3 = \frac{1}{\sqrt{3}} (\underset{\sim}{x}_1 + \underset{\sim}{x}_2 + \underset{\sim}{x}_3) \tag{1}$$

One notices immediately that the harmonic oscillator Hamiltonian is invariant under the change from single particle coordinates $\underset{\sim}{x}_i$ to the more convenient $\dot{\underset{\sim}{x}}_i$. Since our nucleon-nucleon potential is translationally invariant, we may drop the coordinate $\underset{\sim}{x}_3$ and may write a complete set of orbital states for the three-body system as

$$|\phi_{\dot{n}_1\dot{\ell}_1}(\dot{\underset{\sim}{x}}_1)\phi_{\dot{n}_2\dot{\ell}_2}(\dot{\underset{\sim}{x}}_2)LM\rangle = A_{\dot{n}_1\dot{\ell}_1} A_{\dot{n}_2\dot{\ell}_2} (\dot{\underset{\sim}{\eta}}_1 \cdot \dot{\underset{\sim}{\eta}}_1)^{\dot{n}_1} (\dot{\underset{\sim}{\eta}}_2 \cdot \dot{\underset{\sim}{\eta}}_2)^{\dot{n}_2}$$

$$\times [Y_{\dot{\ell}_1}(\dot{\underset{\sim}{\eta}}_1)\, Y_{\dot{\ell}_2}(\dot{\underset{\sim}{\eta}}_2)]_{LM}|0\rangle \tag{2}$$

where the $A_{n\ell}$ are normalization constants, $|0\rangle$ is the harmonic oscillator ground state, and the $\dot{\underset{\sim}{\eta}}_i$ are the usual harmonic oscillator creation operators which have the form

$$\dot{\underset{\sim}{\eta}}_j = \frac{1}{\sqrt{2}} (\dot{\underset{\sim}{x}}_j - i\dot{\underset{\sim}{p}}_j) \quad . \tag{3}$$

Both Jahn[4] and Moshinsky, et al.[2] have shown that it is a relatively simple matter to construct orbital states having well-defined particle permutation symmetry as a sum of terms of the form (2) subject only to the constraint that the total number of oscillator quanta

$$Q = (2n_1 + \ell_1) + (2n_2 + \ell_2) \tag{4}$$

be constant. This restriction is due to the fact that the oscillator Hamiltonian commutes with the particle permutation operators. We shall now summarize the arguments of reference 2 where it is shown that the coefficients in such an expansion are closely related to the ordinary harmonic oscillator transformation brackets.[5]

We first define a transformation of the creation operators

$$\begin{aligned} \underset{\sim}{\eta}_1 &= \frac{1}{\sqrt{2}}(-i\dot{\underset{\sim}{\eta}}_1 + \dot{\underset{\sim}{\eta}}_2) \\ \underset{\sim}{\eta} &= \frac{1}{\sqrt{2}}(+i\dot{\underset{\sim}{\eta}}_1 + \dot{\underset{\sim}{\eta}}_2) \end{aligned} \tag{5}$$

The operators $\underset{\sim}{\eta}_i$ have the following behavior under the application of the particle permutation operators (1,2) and (1,2,3)

$$(1,2)\begin{pmatrix} \underset{\sim}{\eta}_1 \\ \underset{\sim}{\eta}_2 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} \underset{\sim}{\eta}_1 \\ \underset{\sim}{\eta}_2 \end{pmatrix}$$

$$(1,2,3)\begin{pmatrix} \underset{\sim}{\eta}_1 \\ \underset{\sim}{\eta}_2 \end{pmatrix} = \begin{pmatrix} e^{\frac{-2\pi i}{3}} & 0 \\ 0 & e^{\frac{2\pi i}{3}} \end{pmatrix}\begin{pmatrix} \underset{\sim}{\eta}_1 \\ \underset{\sim}{\eta}_2 \end{pmatrix} \tag{6}$$

The projection operators onto states of orbital permutation symmetry $[\lambda]r$ in the usual Young-Yamanouchi notation may be written as

$$\theta_{[3]} = \frac{1}{6}\,[\underset{\sim}{1} + (1,2) + (1,3) + (2,3) + (1,2,3) + (1,3,2)]$$

$$\theta_{[111]} = \frac{1}{6}\,[\underset{\sim}{1} - (1,2) - (1,3) - (2,3) + (1,2,3) + (1,3,2)]$$

$$\theta_{[21]211} = \frac{1}{6}\,[2\,\underset{\sim}{1} - (1,2,3) - (1,3,2)][\underset{\sim}{1} + (1,2)]$$

$$\theta_{[21]121} = \frac{1}{6}\,[2\,\underset{\sim}{1} - (1,2,3) - (1,3,2)][\underset{\sim}{1} - (1,2)] \tag{7}$$

We now write oscillator states in terms of the new creation operators $\underset{\sim}{\eta}_i$ in a manner completely analogous to equation (5).

$$\left\{ |\phi_{n_1\ell_1}\phi_{n_2\ell_2}\, L\rangle + (-)^{\ell_1+\ell_2-L+\tau}\, |\phi_{n_2\ell_2}\phi_{n_1\ell_1}\, L\rangle \right\} \tag{8}$$

From the definitions of the projection operators (7) and the behavior of the creation operators under the permutations (1,2) and (1,2,3) it is straightforward to show that the states given by equation (8) are states of well-defined permutation symmetry. To assist in classifying these states it is convenient to introduce the index ν defined as

$$\nu(\mathrm{mod}\ 3) = 2n_1 + \ell_1 - 2n_2 - \ell_2 \quad . \tag{9}$$

The connection between ν, n_i, ℓ_i, and τ and the permutation symmetry $[\lambda]r$ of the states of equation (8) is given in Table 1.

It is now desirable to transform the states (8) into a sum of terms of the form of equation (2) since the latter are far more convenient for numerical calculation. To do this we note that the transformation of the creation operators (5) is identical to the normal Moshinsky transformation[5] except for the additional factor of i. This alteration does nothing more than introduce a modified set of phases. The states of equation (8) may thus be written as

$$|n_1\ell_1 n_2\ell_2 L[\lambda]r\rangle = \sum_{\dot{n}} [n_1\ell_1 n_2\ell_2 L[\lambda]r\,\{\,|\dot{n}_1\dot{\ell}_1\dot{n}_2\dot{\ell}_2]\ |\dot{n}_1\dot{\ell}_1\dot{n}_2\dot{\ell}_2 L\rangle \tag{10}$$

where

$$[n_1\ell_1 n_2\ell_2 L[\lambda]r \{|\dot{n}_1\dot{\ell}_1\dot{n}_2\dot{\ell}_2] = A(\nu,\lambda,r)[1+(-)^{\tau+\dot{\ell}_1}](-)^{\dot{n}_1+\dot{\ell}_1}$$

$$\times\, i^{\dot{\ell}_1} \langle \dot{n}_1\dot{\ell}_1\dot{n}_2\dot{\ell}_2 \{|n_1\ell_1 n_2\ell_2 L\rangle \quad . \tag{11}$$

The quantities $\langle n_1\ell_1 n_2\ell_2 \{|n_1\ell_1 n_2\ell_2\rangle$ are the ordinary harmonic oscillator transformation brackets and τ and $A(\nu,\lambda,r)$ are given in Table 1.

We have thus completed the initial task of constructing a complete set of orbital states having permutation symmetry $[\lambda]r$. We shall label these states as $|n_1\ell_1 n_2\ell_2 L[\lambda]r\rangle$. Totally antisymmetric states may be obtained with the introduction of spin-isospin states of adjoint symmetry $[\tilde{\lambda}]\tilde{r}$ as constructed by Jahn[6] and by Kramer and Moshinsky[7]. The totally antisymmetric states have the form

$$|n_1\ell_1 n_2\ell_2 LSJT[\lambda]\rangle = \frac{1}{\sqrt{f_{[\lambda]}}} \sum_J (-)^r [|n_1\ell_1 n_2\ell_2 L[\lambda]r\rangle |ST[\tilde{\lambda}]\tilde{r}\rangle]^J \tag{12}$$

where $f_{[3]}$ and $f_{[111]}$ are 1 and $f_{[21]}$ is 2. The phase $(-)^r$ is defined to be positive except when r = 121 when it is negative.

Matrix elements of the nucleon-nucleon potential in the basis $|n_1\ell_1 n_2\ell_2 LSJT[\lambda]\rangle$ can now be easily evaluated. We note for convenience that the matrix elements of the full two-body potential $\sum_{i<j} V(\underset{\sim}{r}_{ij})$ in this antisymmetrized basis will be identical to the matrix elements of 3 $V(\underset{\sim}{\dot{x}}_1)$. The latter are, of course, more easily evaluated.

It is often desirable to simplify an actual triton calculation with the assumption that the nucleon-nucleon potential only acts in a restricted number of partial waves. This restriction will simplify the calculation only if the matrix elements of the kinetic energy operator, which acts in all partial wave channels, can be determined without the explicit use of transformation brackets. In fact, the kinetic energy matrix elements can be evaluated easily. When the number of quanta is unchanged one finds

$$\langle n_1\ell_1 n_2\ell_2 LSJT[\lambda]|\underline{T}|n_1\ell_1 n_2\ell_2 LSJT[\lambda']\rangle = \frac{1}{2}(2n_1 + \ell_1 + 2n_2 + \ell_2 + 3)\hbar\omega\,\delta_{[\lambda][\lambda']} \tag{13}$$

When the number of quanta on left and right sides of the matrix element differ by 2, the matrix elements of the kinetic energy operator may be calculated with the aid of the recursion relations for harmonic oscillator transformation brackets given by Brody and Moshinsky[5]. For example, for states of symmetry [3] the matrix elements of the kinetic energy operator are

$$(-)^{\ell_2+\ell'_2}\left[\frac{\langle n_2\ell_2 n_1\ell_1 L|-r_1^2|n'_1\ell'_1 n'_2\ell'_2 L\rangle + \langle n_1\ell_1 n_2\ell_2 L|-r_1^2|n'_1\ell'_1 n'_2\ell'_2 L\rangle}{\sqrt{1+\delta_{n_1 n'_1}\delta_{\ell_1\ell'_1}}\qquad\qquad\sqrt{1+\delta_{n_2 n'_2}\delta_{\ell_2\ell'_2}}}\right] \tag{14}$$

For states of symmetry [21] with $\nu+\nu'$ odd the matrix elements are

$$2(-)^{\ell_2+\ell'_2}\langle n_1\ell_1 n_2\ell_2 L|-r_1^2|n'_1\ell'_1 n'_2\ell'_2 L\rangle \tag{15}$$

For states of symmetry [21] with $\nu+\nu'$ even one obtains the same expression as (15) except for the interchange of $n_1\ell_1$ with $n_2\ell_2$. The matrix elements $\langle n_1\ell_1 n_2\ell_2 L|-r_1^2|n'_1\ell'_1 n'_2\ell'_2 L\rangle$ are tabulated in reference 5.

We have introduced a systematic way to generate a complete set of antisymmetric three-body states in a basis convenient for calculation. We can now construct and diagonalize the Hamiltonian matrix including all states with Q less than some Q_0. If the details of the potential permit, we may also eliminate certain orbital permutation symmetries from the calculation. For example, if the $^1S_0$ and $^3S_1$ interactions are equal, the triton ground state will contain no [21]S component. The choice of Q_0 will depend on the details of the nucleon-nucleon potential under consideration. It is not yet clear that a value of Q_0 sufficiently small to permit a calculation will be sufficiently large to provide a good description of the triton wave function for realistically hard nucleon-nucleon potentials. We note that this technique makes use of the harmonic

oscillator matrix elements of the two-body potential and thus cannot be used to calculate the triton binding energy with hard core potentials.

III. Yamaguchi potential

As a test of the practical value of this technique we calculate the triton binding energy using the Yamaguchi potential.[8] This potential is constructed to act only in singlet-S and triplet-S states. Each potential is a single term separable potential having the form

$$\langle p|V_S|p'\rangle = -\frac{\lambda_S}{M}\,\frac{1}{p^2+\beta^2}\,\frac{1}{p'^2+\beta^2} \tag{16}$$

These potentials provide a satisfactory description of low energy phase shifts but are not designed to fit higher energy scattering data. The Yamaguchi potential is not realistic, but it does have the advantage of being separable. We can thus compare the triton binding energy obtained according to the prescription given in the preceding section with the exact result obtained from a solution of the Faddeev equations.

We have performed the calculation with the simplifying assumption that the singlet-S and triplet-S interactions are equal to their average. The potential parameters are thus $\lambda = 0.35249\ f^{-3}$ and $\beta = 1.4487\ f^{-1}$. Since [21]S states are built into the triton ground state by the difference between these potentials, this assumption is equivalent to the restriction to [3]S states. Matrix elements of this potential in a relative oscillator basis are simply related to the error function. Oscillator matrix elements for large radial quantum numbers may be obtained more simply by replacing the harmonic oscillator wave functions with appropriately chosen bessel functions.[9] The triton binding energy is shown in Figure 1 as a function of Q_0. Calculations were performed for a number of values of $\hbar\omega$, and fastest convergence was obtained for $\hbar\omega = 64.79$ MeV. For $Q_0 = 28$ the Hamiltonian matrix included 147 [3]S states, and the triton binding energy was found to be 12.19 MeV. This result is in satisfactory agreement with

the value of 12.49 ± 0.01 MeV obtained by Hartt by solving the Faddeev equations for the same potential.[10]

In hope of providing some insight into the rate of convergence of the triton binding energy, we consider an oscillator calculation of the deuteron binding energy. This is a much simpler problem since there exists only one $^3S_1$ state for each even value of Q and, when tensor forces are present, one $^3D_1$ state for each value of Q greater than zero. The deuteron binding energy for $\hbar\omega$ = 51.10 MeV is shown as a function of Q_0 in Figure 2. At Q_0 = 28 the deuteron binding energy is 1.87 MeV which is 82% of the correct value. It is tempting to suggest that the rate of convergence of the deuteron binding energy may serve as a measure of the convergence of the more complicated three-body calculation. This is not unreasonable since the role of components having large Q is to build in the short range correlations caused by the repulsive core of a realistic potential and to build up the proper exponentially decaying tail from the gaussian behavior of the individual components. It is hoped that neither of these effects should be particularly sensitive to the number of nucleons present. Since the triton is bound more tightly than the deuteron, it is even possible that the triton binding energy calculation may converge more rapidly than the corresponding deuteron calculation. We note that a deuteron calculation with a separable potential of the form (16) chosen to give a two-body binding energy of 8.0 MeV converged to 95% of the true binding energy with Q_0 = 28.

On the basis of a comparison of our triton results with the Faddeev equation results of Hartt, we conclude that this systematic technique for the generation of a triton wave function is capable of providing meaningful results with a practical number of states in the basis. Furthermore, we suggest that a shell model deuteron calculation with the same potential can yield some measure of the rate of convergence of the three-body binding energy.

IV. Reid Potential

A more rigorous test of this method comes from a calculation of the triton binding energy with the Reid potential.[11] The Reid potential is a superposition of Yukawa potentials which provides and essentially quantitative fit to scattering data for laboratory energies less than 350 MeV. It contains strong but finite short range repulsions and certainly qualifies as a realistic potential. Harmonic oscillator matrix elements of the Reid potential were calculated in terms of parabolic cylinder functions. Oscillator matrix elements with large radial quantum numbers could again be approximated by replacing harmonic oscillator wave functions with appropriate bessel functions.[9] We anticipate initially that the binding energy calculation with the Reid potential will be more difficult than the preceding separable potential calculation. When Q_0 equals 0 the Yamaguchi potential used in Section III yields a triton unbound by about 6 MeV. A similar calculation with the Reid potential results in a triton unbound by approximately 700 MeV. The calculation is further complicated by the fact that the Reid potential contains a strong tensor component which demands the inclusion of [21]D states. The $^1S_0$ and $^3S_1$ interactions are no longer equal and we can no longer be confident in excluding [21]S states.

To gain some feeling for the value of Q_0 at which we might expect to obtain a reliable estimate of the binding energy, we again consider the analogous deuteron calculation. The deuteron binding energy is shown in Figure 3 for $\hbar\omega$ = 51.19 MeV as a function of Q_0. For Q_0 = 48 we find a deuteron binding energy of 2.11 MeV, a quadrupole moment of 0.282 f^2, and a D-state probability of 6.5%. These results are in good agreement with the exact values of 2.225 MeV, 0.280 f^2, and 6.5% respectively. At Q_0 = 28 the binding energy is 1.86 MeV, the quadrupole moment is 0.243 f^2 and the D-state probability is 6.8%. It is surprising to note that the convergence of the deuteron binding energy is essentially the same for the Reid potential and for the Yamaguchi potential. It

is thus to be hoped that the triton calculation will show convergence properties similar to those obtained with the Yamaguchi potential.

Since the number of [21]D states grows rapidly with Q_0, it was not numerically practical to treat the [3]S states and [21]D states in an equivalent manner. (For example, at $Q_0 = 16$ there are 41 [3]S states and 120 [21]D states. At $Q_0 = 28$ there are 147 [3]S states and 560 [21]D states.) In the interest of further simplifying the calculation we have also neglected states of all other permutation symmetries. The neglect of [21]S states is probably not justified for the Reid potential as they are expected to contribute approximately 1 MeV to the triton binding energy.[12] The nucleon-nucleon interaction was assumed to act only in the $^1S_0$, $^3S_1$, $^3S_1$-$^3D_1$, and $^3D_1$ channels. The results of triton calculations subject to these restrictions are shown in Table 2 for several values of Q_s and Q_d all less than the desired value of 28. While it is clear that we have not yet obtained convergence at $Q_s = 28$ and $Q_d = 16$, the calculated binding energy of 3.86 MeV is a significant result.

This result may be compared with the triton binding energy of 6.8 MeV obtained by Delves, et al.[1] with the Hamada-Johnston potential. Tjon has obtained a value of 6.5 ± 0.1 MeV for the Reid potential using an elegant iterative solution to the Faddeev equations.[12] Tjon includes the effects of [21]S states, but makes the same restrictions on the two-nucleon potential.

Calculations are in progress to increase Q_s and Q_d, to include the effects of states having other permutation symmetry, and to include the effects of higher partial waves of the nucleon-nucleon interaction. Nonetheless, it is already clear that this straight forward approach to the three-body problem is a practical one and is capable of providing meaningful results even for realistic potentials.

Acknowledgments

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TABLE I

$[\lambda]r$	ν	τ	$A(\nu, [\lambda]r)$
[3]	0 $n_1 \neq n_2$ $\ell_1 \neq \ell_2$	0	$1/\sqrt{2}$
[3]	0 $n_1 = n_2$ $\ell_1 = \ell_2$ L even	0	$1/2$
[21] 211	1,2	0	$1/\sqrt{2}$
[21] 121	1,2	1	$(-i)(-)^{\nu}/\sqrt{2}$
[111]	0 $n_1 \neq n_2$ $\ell_1 \neq \ell_2$	1	$1/\sqrt{2}$
[111]	0 $n_1 = n_2$ $\ell_1 = \ell_2$ L odd	1	$1/2$

TABLE II

Q_S	Q_D	$\hbar\omega$ (MeV)	B (MeV)	T (MeV)	[21] D %
28	10	41.47	.78	59.85	7.30
20	16	41.47	1.61	60.96	7.83
26	12	41.47	1.75	62.59	7.86
24	14	41.47	2.21	63.36	7.80
24	14	64.79	2.79	89.83	8.95
24	14	51.19	3.03	74.88	8.43
28	16	51.19	3.81	.....	....

Figure Captions

Figure 1. Triton binding energy in MeV as a function of the maximum number of quanta Q_0 for the Yamagouchi potential. Dashed line represents Faddeev equation result.

Figure 2. Deuteron binding energy in MeV as a function of the maximum number of quanta Q_0 for the Yamagouchi potential. Dashed line represents exact value.

Figure 3. Deuteron binding energy in MeV as a function of the maximum number of quanta Q_0 for the Reid potential. Dashed line represents exact value.

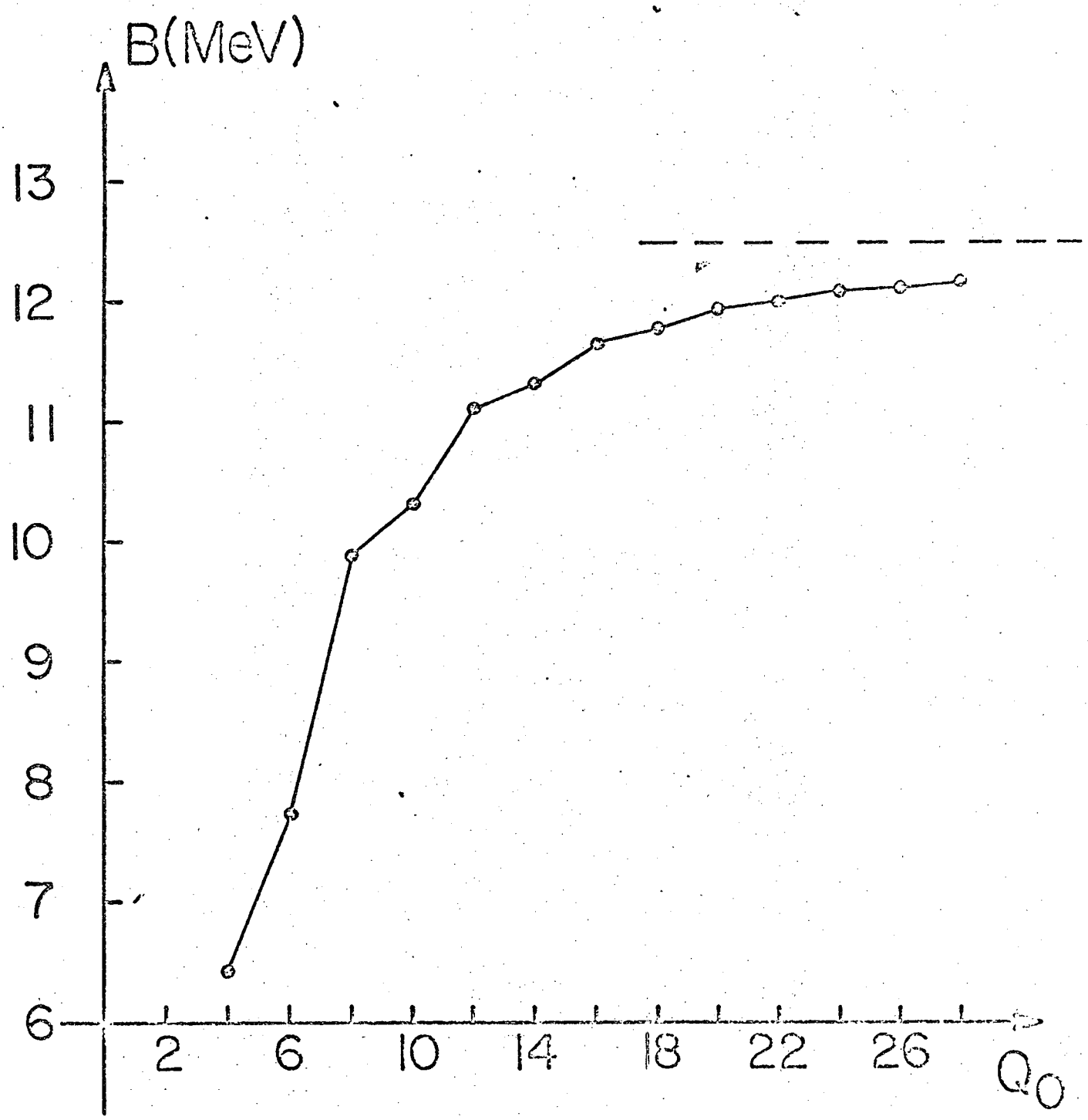

Fig. 1

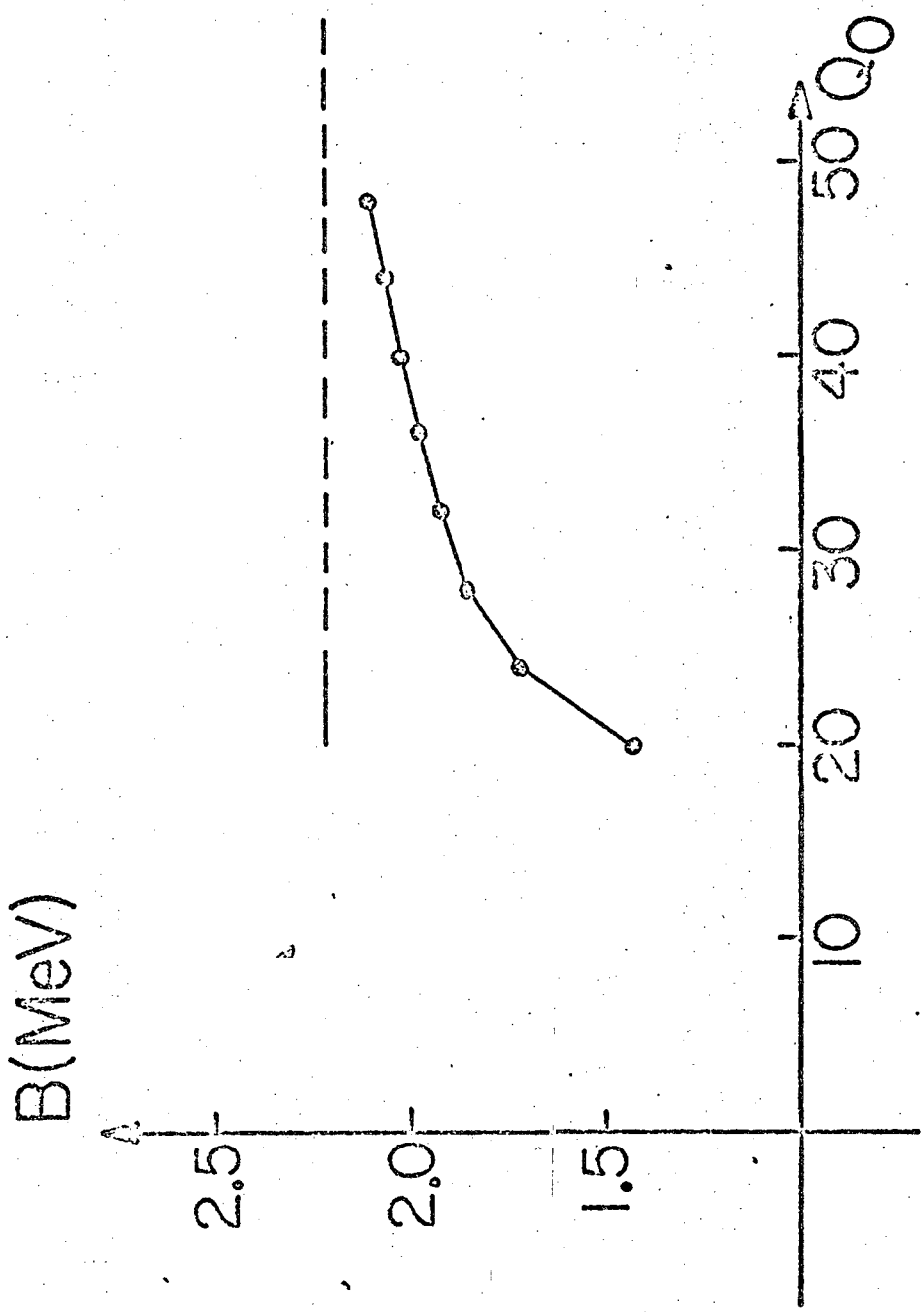

Fig. 2

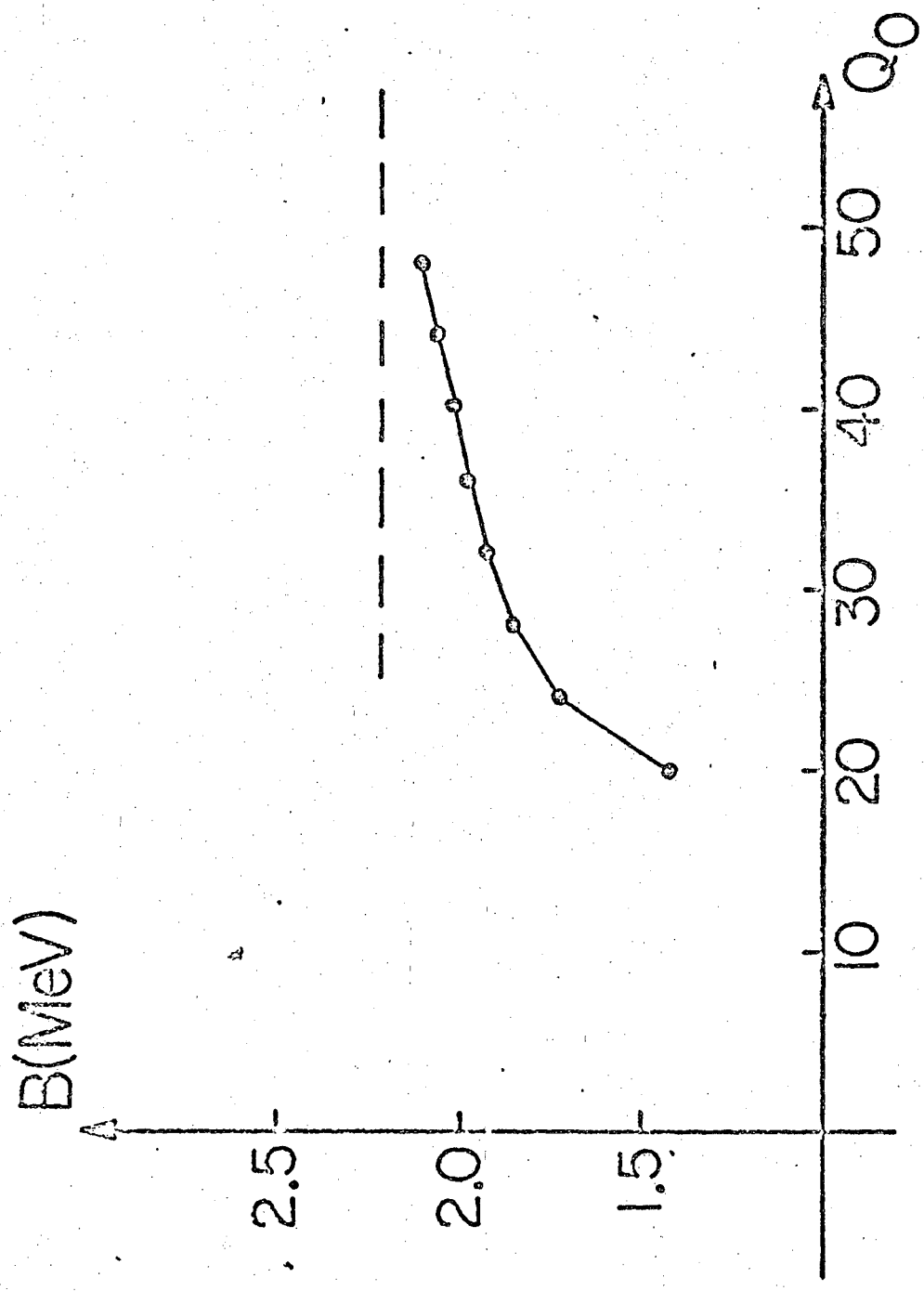

Fig. 3

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