Quantum exchange effects in trimer ground states[a),b)]

M. L. Cramer,[c)] L. W. Bruch, and F. Cabral[d)]

Department of Physics, University of Wisconsin-Madison, Madison, Wisconsin 53706
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The ground state of molecular trimers is studied in three dimensions for these pair potential models: the square well, the exponential, the Yukawa, the Gaussian, and the Lennard-Jones 12–6. Three spin cases are considered: three spin-zero bosons and the spin-(1/2) and spin-(3/2) states of three spin-(1/2) fermions. Variational wavefunctions are constructed which satisfy the exchange symmetry requirements for these cases. Bounds are obtained for the threshold coupling constants at which self-bound trimers occur. Consequences for possible self-bound trimers of ^{3}He are discussed.

I. INTRODUCTION

In quantum mechanics, particles are classed as bosons or fermions and accordingly their states show different symmetries under exchange of particle labels. The consequences are readily observed even for atoms, as in the mutual scatterings[1] of helium atoms or of neon atoms. Here we treat exchange effects between such massive objects near the threshold for three-particle, or trimer, self-binding.

We study the ground state of three identical particles in three dimensions interacting via central pair potentials. As models for the pair potential we use the square well, the exponential well, the Yukawa well, the Gaussian well, and the Lennard-Jones 12–6 potential. The first four models are coreless potentials[2] for which we have variational wavefunctions for which the energy expectation value can be reduced analytically and which locate the threshold coupling constants within narrow ranges. We use results obtained for these models as guides in the treatment of the Lennard-Jones model, which is a useful model for inert gas trimers.

The inert gas trimers for which self-binding is in doubt[3] are trimers of the fermion isotope of helium, ^{3}He, and we use our results for the Lennard-Jones model to reinforce an earlier conclusion[3] that self-bound ^{3}He trimers are unlikely.

The corresponding question in nuclear physics is on the occurrence of a bound trineutron[4]; our treatment is simpler because in the nuclear case there are significant spin-dependent forces to be included.

In Sec. II we present our results for the boson trimer for the coreless potentials; the Lennard-Jones model has been treated elsewhere.[3] In Sec. III we give a general discussion of the effect of exchange symmetry requirements on the ground state of the fermion trimer. Sections IV and V contain the results of variational calculations for the spin-(1/2) and spin-(3/2) fermion trimers with coreless potentials. The results of Secs. II, IV, and V are collected in Tables I and II and are appraised in Sec. VI. Then we present our results for the Lennard-Jones fermion trimers in Sec. VII and a final discussion in Sec. VIII. An Appendix is included which contains a review of the group theoretical treatment of the states of three particles in a rigid equilateral triangle configuration.

II. BOSON TRIMER: CORELESS POTENTIALS

Most attempts[3,5–9] at evaluating the ground state energy of inert gas trimers have used variational methods. For three spin-zero bosons, the trial wavefunctions have been of zero total angular momentum[10] and have usually been of the Jastrow form.

We have found[11] that for three spin-zero bosons interacting via central coreless pair potentials a useful variational wavefunction is[12]

$$\psi(1,\ 2,\ 3) = N \exp[-\alpha(r_{12} + r_{23} + r_{31})]\ , \tag{1}$$

where r_{ij} are the interparticle distances and N is a normalization constant. The Rayleigh–Ritz expectation value for this function can be found analytically, the function has the qualitatively correct exponential behavior at large interparticle separations, and near the threshold for self-binding it yields a lower energy than a product of Gaussians.

We have calculated the expectation value of the kinetic energy operator

$$K = -(\hbar^2/2m)(\nabla_1^2 + \nabla_2^2 + \nabla_3^2) \tag{2}$$

for three particles of mass m with Eq. (1), using ordinary Cartesian coordinates, and find

$$\langle K\rangle = (30/7)\hbar^2\alpha^2/m\ . \tag{3}$$

The four coreless central pair potential models which we consider are[2]

$$\text{(A) Square well:}\quad V_s(r) = \begin{cases} -V_0 & r < r_0 \\ 0 & r \geq r_0\ ; \end{cases} \tag{4}$$

$$\text{(B) Exponential well:}\quad V_e(r) = -V_0 \exp(-r/r_0)\ ; \tag{5}$$

$$\text{(C) Yukawa well:}\quad V_y(r) = -V_0(r_0/r)\exp(-r/r_0)\ ; \tag{6}$$

$$\text{(D) Gaussian well:}\quad V_G(r) = -V_0 \exp(-r^2/r_0^2)\ . \tag{7}$$

For all of these we define dimensionless variational parameters x and coupling constants K by

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[c)]Present address: The BDM Corporation; 7915 Jones Branch Dr.; McLean, VA 22101.

[d)]Supported in part by Universidade Federal de Santa Catarina through the U. S. A. I. D.-Brazil Program.

TABLE I. Threshold coupling constants for self-binding.

	Two body			Three body	
Pair model[a]	A. $K_c(l=0)$	B. $K_c(l=1)$	C. $K_c^{\mu b}(l=0)^{f}$	D. $K_c^{\mu b}\binom{l=1}{s=1/2}^{g}$	E. $K_c^{\mu b}\binom{l=1}{s=1/2}^{h}$
Square well	$\frac{\pi^2}{4}=2.4674^{b}$	$\pi^2=9.8696^{b}$	2.096023	4.077222	7.238101
Exponential	1.446[c]	7.049[e]	1.222041	2.373106	5.021898
Yukawa	1.67982[d]	9.082[e]	1.462678	2.834612	6.655844
Gaussian	2.684[e]	12.100[e]	2.247772	4.368196	8.896328

[a]Models defined in Eqs. (4)–(7) of text, coupling K defined in Eq. (9).
[b]From analytical solution of the Schrödinger equation.
[c]From analytical solution in terms of zero of a Bessel function, Ref. 2.
[d]References 2 and 13.
[e]Values obtained by our numerical solution of the Schrödinger equation.
[f]Upper bound for three boson threshold, obtained as described in Sec. II.
[g]Upper bound for spin-(1/2) threshold of three spin-1/2 fermions, obtained as described in Sec. IV.
[h]Upper bound for spin-(3/2) threshold of three spin-1/2 fermions, obtained as described in Sec. V.

$$x=4\alpha r_0\,, \tag{8}$$

$$K=mr_0^2V_0/\hbar^2\,. \tag{9}$$

Taking the expectation value of the potential energies with the trial function Eq. (1), adding the kinetic energy Eq. (3), and using the definitions Eqs. (8) and (9), we find upper bounds on the ground state energy: for the square well,

$$\frac{E}{3V_0}=\frac{5}{56}\left(\frac{x^2}{K}\right)-1+\left(\frac{x^4}{84}+\frac{5x^3}{42}+\frac{x^2}{2}+x+1\right)e^{-x}\,; \tag{10}$$

for the exponential well,

$$\frac{E}{3V_0}=\frac{5}{56}\left(\frac{x^2}{K}\right)-\left(\frac{2}{7}\,\frac{x^5}{(1+x)^5}+\frac{3}{7}\,\frac{x^4}{(1+x)^4}+\frac{2}{7}\,\frac{x^3}{(1+x)^3}\right)\,; \tag{11}$$

for the Yukawa well,

$$\frac{E}{3V_0}=\frac{5}{56}\left(\frac{x^2}{K}\right)-\left(\frac{x^5}{14(1+x)^4}+\frac{x^4}{7(1+x)^3}+\frac{x^3}{7(1+x)^2}\right)\,; \tag{12}$$

and for the Gaussian well,

$$\frac{E}{3V_0}=\frac{5}{56}\left(\frac{x^2}{K}\right)-\left\{(-)\frac{4}{21}\left(\frac{x}{2}\right)^8+\frac{2}{21}\left(\frac{x}{2}\right)^6+\left[\frac{4}{21}\left(\frac{x}{2}\right)^9-\frac{1}{7}\left(\frac{x}{2}\right)^5+\frac{2}{7}\left(\frac{x}{2}\right)^3\right]\sqrt{\pi}\,e^{x^2/4}\left[1-\mathrm{erf}\left(\frac{x}{2}\right)\right]\right\}, \tag{13}$$

where $\mathrm{erf}(z)$ is the error function $\mathrm{erf}(z)=(2/\pi^{1/2})\int_0^z e^{-t^2}\,dt$.

For given coupling constant K, the variational energies were minimized as a function of the parameter x and the values of K at which the variational energy first becomes negative were found. Since for each potential the variational energy is an upper bound to the exact ground state energy, this procedure gives upper bounds to the threshold coupling constants for self-binding. We analyzed Eqs. (10)–(13) numerically and our results are entered in Column C of Table I.

Columns A and B of Table I are threshold coupling constants[2,13] for two-body states of zero and one unit of angular momentum. They are used in forming the reduced threshold constants which are presented in Table II and discussed in Sec. VI. Column G is the ratio of Column C to Column A: Hall and Post[14] proved the values in Column G must be larger than $\frac{2}{3}$; Bruch and Sawada[15] showed that the exact (true) ratios for three bosons must be less than 1. Column G is an upper bound on the exact values and represents a considerable improvement on the Bruch–Sawada upper bound.

III. FERMION TRIMER EXCHANGE REQUIREMENTS

We consider trimers composed of three identical spin-(1/2) particles. As these are fermions and obey Fermi-Dirac statistics, the total trimer wavefunction must be antisymmetric under pair exchange and symmetric under three-cycle exchanges.

We construct trimer wavefunctions in which the spatial components have one unit of angular momentum, P states. It is possible to construct wavefunctions for the fermion trimer of zero spatial angular momentum but we have made our variational search for the threshold of fermion trimer self-binding in P states for several reasons: (1) By analogy with the two-body problem, it is plausible that the wavefunction nodes required by the antisymmetry can be introduced with the least increase of energy by rotational motion rather than by the excitation of relative motion of the particles. (2) In the semi-

TABLE II. Trimer threshold coupling constants in reduced form.

Pair model[a]	F[b]. $\frac{B}{A}$	G.[b] $\frac{C}{A}$	H[b]. $\frac{D}{A}$	I[b]. $\frac{E}{A}$	J[b]. $\frac{D}{B}$	K[b]. $\frac{E}{B}$
Square well	4.000	0.849	1.652	2.933	0.413	0.733
Exponential	4.875	0.845	1.641	3.473	0.337	0.713
Yukawa	5.407	0.871	1.688	3.962	0.312	0.733
Guassian	4.508	0.838	1.628	3.315	0.361	0.735

[a]Models defined in Eqs. (4)–(7) of text.
[b]Entries in these columns are ratios of entries in the designated columns of Table I; for discussion see Sec. VI.

classical fermion trimers, treated in Appendix A, the lowest states are P states. (3) For the spin-(3/2) trimer, Hall's lower-bound comparison problem[16] has one unit of angular momentum. (4) The nuclear physics model calculations for trineutrons have emphasized P states.[4]

The thresholds we find in the trimer P states are below the thresholds for the dimer P states; then a demonstration that the expectation value of the Hamiltonian is negative relative to the energy of three well-separated particles is sufficient to establish self-binding of the three particles. However, the thresholds we find are above the thresholds for dimer S states, which opens a question whether the spin-(1/2) trial function we use is sufficiently general. In S states the trimer calculations would be more delicate; one would have to establish that the trimer energy is lower than the dimer energy. For three bosons, this is established by the Bruch–Sawada upper bound.[15] Efimov[17] showed for three bosons that there are weakly bound trimer states just below the threshold for dimer binding; he also showed[17] these states do not arise in the mixed symmetry state ($S=1/2$) of three identical spin-(1/2) fermions. That is, there are no Efimov states to prove the spin-(1/2) trimer threshold is below the dimer threshold and the lowest spin-(1/2) trimer bound state is likely to be the P state for the reasons given above. Such questions do not arise for the spin-(3/2) trimer, where we have located the threshold between narrow limits.

A. Spin structure

The trimer wavefunction is composed of spatial and spin parts. If the spins align, the trimer has spin-(3/2) and the spin representation comes from the spin quartet. If the spins do not all align, the trimer has spin-(1/2) and the spin representation comes from each of two possible spin doublets, hence the reference to the spin-(1/2) case as the "mixed-symmetry" trimer. One doublet, X_s, can be constructed[16] to be symmetric and the other doublet, X_a, to be antisymmetric under the interchange of particles one and two.

Explicitly, the $+1/2$ projections of the doublets are

$$X_a(s_z=1/2)=(1/\sqrt{2})(\alpha_1\beta_2\alpha_3-\beta_1\alpha_2\alpha_3)\,, \tag{14}$$

$$X_s(s_z=1/2)=(1/\sqrt{6})(2\alpha_1\alpha_2\beta_3-\alpha_1\beta_2\alpha_3-\beta_1\alpha_2\alpha_3)\,,$$

where the $\alpha(\beta)$ are the usual spin up (down) eigenstates of a spin-(1/2) particle and the subscripts are the particle labels.

B. Parity

We require that ψ be a parity eigenstate,[18] i.e.,

$$P\psi=\pm\psi\,. \tag{15}$$

The effect of parity is only on the spatial orientation of the triangular configuration of the three particles; the interparticle distances remain unchanged.

The rigid-rotor wavefunctions[18,19] $D^l_{mm'}(\alpha,\beta,\gamma)$, in which l is the total angular momentum quantum number, m is a space-axis projection, and m' is a body-axis projection, provide a set of angular momentum states with parity eigenvalue $(-1)^{m'}$. In an expansion of a three-particle wavefunction ψ using these states, the requirement that ψ be a parity eigenstate means that only even or only odd m' appear.[19]

C. Spin-(3/2) trimer

The spin part X of the spin-(3/2) trimer wavefunction comes from the spin quartet, each member of which is invariant under three-cycle exchanges and pair exchanges. Thus the remaining factors of the wavefunction must be antisymmetric under pair exchanges. The wavefunction is factored

$$\psi=\phi^l_m X\,, \tag{16}$$

and expanded

$$\phi^l_m=\sum_{m'=-l}^{l} g^l_{m'}D^l_{mm'}\,. \tag{17}$$

The $g^l_{m'}$ are functions of the interparticle distances.

We are guided by the special case of the equilateral triangle[20] treated in Appendix A to construct a trial function with $l=1$ and retaining only the $m'=0$ component. This is a parity eigenstate.

D. Spin-(1/2) trimer

For the mixed-symmetry trimer, we must modify Eqs. (16) and (17) to allow for the construction of ψ from both of the spin doublets,[16] Eq. (14),

$$\psi=\phi_a X_s+\phi_s X_a\,; \tag{18}$$

ϕ_a and ϕ_s are antisymmetric and symmetric, respectively, under the pair exchange of one and two, so that ψ is antisymmetric under the one–two exchange.

Applying pair exchange, P_{12}, and cyclic exchange, C_{123}, to the spin doublets of Eq. (14) we have

$$P_{12}X_s=X_s\,,$$

$$C_{123}X_s=(-)\tfrac{1}{2}X_s+\tfrac{1}{2}\sqrt{3}X_a\,; \tag{19}$$

$$P_{12}X_a=-X_a\,,$$

$$C_{123}X_a=-\tfrac{1}{2}\sqrt{3}X_s-\tfrac{1}{2}X_a\,. \tag{20}$$

Requiring that ψ in Eq. (18) be antisymmetric under P_{12} and symmetric under C_{123} leads to the relations

$$P_{12}\phi_a=-\phi_a\,,$$

$$C_{123}\phi_a=(-)\tfrac{1}{2}\phi_a+\tfrac{1}{2}\sqrt{3}\phi_s\,; \tag{21}$$

$$P_{12}\phi_s=\phi_s\,,$$

$$C_{123}\phi_s=-\tfrac{1}{2}\sqrt{3}\phi_a-\tfrac{1}{2}\phi_s\,. \tag{22}$$

As in the spin-(3/2) case we construct a trial function with one unit of angular momentum:

$$\phi_s=a_1D^1_{m1}+a_0D^1_{m0}+a_{-1}D^1_{m-1}\,, \tag{23}$$

$$\phi_a=b_1D^1_{m1}+b_0D^1_{m0}+b_{-1}D^1_{m-1}\,.$$

The a_i and b_i in Eq. (23) are functions of the internal coordinates. We cannot mix even and odd parity components. From the equilateral triangle case[20] in Appendix A, we are led to choose $a_0=b_0=0$ in the variational trial function for the spin-(1/2) trimer ground state.

IV. SPIN-(1/2) TRIMER VARIATIONAL CALCULATION

We now construct a trial function meeting the requirements of Sec. III. D. and based on the boson trial function Eq. (1). We are to construct functions ϕ_a and ϕ_s, Eq. (17), satisfying Eqs. (21) and (22). Guidance is provided by inspection of the exactly known excited states of three particles interacting through Hooke's law pair potentials,[14]

$$V(r_{ij}) = \tfrac{1}{2} k r_{ij}^2 / 2 \,. \tag{24}$$

As is apparent from Eq. (23), there is some arbitrariness in the construction, reflecting the space-quantization degeneracy of nonzero angular momentum. We take for the functions ϕ_a and ϕ_s

$$\phi_a = (z_1 - z_2)\, e^{-\alpha(r_{12}+r_{23}+r_{31})} \tag{25}$$

and

$$\phi_s = \frac{1}{\sqrt{3}} \left[(z_3 - z_1) - (z_2 - z_3)\right] e^{-\alpha(r_{12}+r_{23}+r_{31})} \,. \tag{26}$$

With these in Eq. (17), we have a trial function for the spin-(1/2) trimer that can be rewritten in terms of the functions D^1_{01} and D^1_{0-1} by transforming from space-fixed to body-fixed axes.[21]

Using Eq. (2), the kinetic energy is found to be

$$\langle K \rangle = \frac{\hbar^2 \alpha^2}{M} \frac{77}{18} = \frac{77}{288} \frac{x^2}{K} V_0 \,. \tag{27}$$

We again consider the coreless, pair potentials, Eqs. (10)–(13), take the expectation value of the potential energies with the spin-(1/2) trial function, add in the kinetic energy Eq. (27) and have as upper bounds on the ground state energy the following: for the square well,

$$\frac{E}{V_0} = \frac{77}{288} \frac{x^2}{K} - \left[3 - \left(\frac{x^6}{1080} + \frac{x^5}{80} + \frac{13x^4}{144} + \frac{4x^3}{9} + \frac{3}{2} x^2 + 3x + 3\right) e^{-x}\right]; \tag{28}$$

for the exponential well,

$$\frac{E}{V_0} = \frac{77}{288} \frac{x^2}{K} - \left(\frac{2}{3} \frac{x^7}{(1+x)^7} + \frac{5}{6} \frac{x^6}{(1+x)^6} + \frac{2}{3} \frac{x^5}{(1+x)^5} + \frac{1}{2} \frac{x^4}{(1+x)^4} + \frac{1}{3} \frac{x^3}{(1+x)^3}\right); \tag{29}$$

for the Yukawa well,

$$\frac{E}{V_0} = \frac{77}{288} \frac{x^2}{K} - \left(\frac{1}{9} \frac{x^7}{(1+x)^6} + \frac{1}{6} \frac{x^6}{(1+x)^5} + \frac{1}{6} \frac{x^5}{(1+x)^4} + \frac{1}{6} \frac{x^4}{(1+x)^3} + \frac{1}{6} \frac{x^3}{(1+x)^2}\right); \tag{30}$$

and for the Gaussian well.

$$\frac{E}{V_0} = \frac{77}{288} \frac{x^2}{K} - \left\{-\frac{8}{135}\left(\frac{x}{2}\right)^{12} - \frac{26}{135}\left(\frac{x}{2}\right)^{10} + \frac{1}{15}\left(\frac{x}{2}\right)^{8} + \left[\frac{8}{135}\left(\frac{x}{2}\right)^{13} + \frac{2}{9}\left(\frac{x}{2}\right)^{11} - \frac{1}{18}\left(\frac{x}{2}\right)^{7} + \frac{1}{3}\left(\frac{x}{2}\right)^{3}\right] \sqrt{\pi}\, e^{x^2/4} \left[1 - \mathrm{erf}\left(\frac{x}{2}\right)\right]\right\}. \tag{31}$$

Equations (28)–(31) were analyzed numerically as in the boson case. The upper bounds on the threshold coupling constants which were found are entered in Column D of Table I.

V. SPIN-(3/2) TRIMER VARIATIONAL CALCULATION

We discussed the wavefunction of the spin-(3/2) trimer in general terms in Sec. III.C. For an explicit trial function we are led, by examination of the excited states of three Hooke's law oscillators, Eq. (24), to choose

$$\phi = (x_1 y_3 - x_3 y_1 + x_2 y_1 - x_1 y_2 + x_3 y_2 - x_2 y_3)\, e^{-\alpha(r_{12}+r_{23}+r_{31})} \tag{32}$$

in space-fixed coordinates. When Eq. (32) is transformed to body-fixed axes[21] the rigid rotor function D^1_{00} appears.

Using Eq. (32), we find the kinetic energy expectation value is

$$\langle K \rangle = \frac{48}{11} \frac{\hbar^2 \alpha^2}{m} = \frac{3}{11} \frac{x^2}{K} V_0 \,. \tag{33}$$

For the coreless potentials, Eqs. (10)–(13), combining the expectation value of potential energy using Eq. (32) with Eq. (33) gives upper bounds on the ground state energy: for the square well,

$$\frac{E}{V_0} = \frac{3}{11}\left(\frac{x^2}{K}\right) - \left[3 - \left(\frac{x^7}{7920} + \frac{19x^6}{7920} + \frac{29x^5}{1320} + \frac{x^4}{8} + \frac{x^3}{2} + \frac{3x^2}{2} + 3x + 3\right) e^{-x}\right]; \tag{34}$$

for the exponential well,

$$\frac{E}{V_0} = \frac{3}{11}\left(\frac{x^2}{K}\right) - \left(\frac{7}{11} \frac{x^8}{(1+x)^8} + \frac{12}{11} \frac{x^7}{(1+x)^7} + \frac{10}{11} \frac{x^6}{(1+x)^6} + \frac{4}{11} \frac{x^5}{(1+x)^5}\right); \tag{35}$$

for the Yukawa well,

$$\frac{E}{V_0} = \frac{3}{11}\left(\frac{x^2}{K}\right) - \left(\frac{1}{11} \frac{x^8}{(1+x)^7} + \frac{2}{11} \frac{x^7}{(1+x)^6} + \frac{2}{11} \frac{x^6}{(1+x)^5} + \frac{1}{11} \frac{x^5}{(1+x)^4}\right); \tag{36}$$

and for the Gaussian well,

$$\frac{E}{V_0} = \frac{3}{11}\left(\frac{x^2}{K}\right) - \left\{\frac{8}{495}\left(\frac{x}{2}\right)^{14} + \frac{32}{495}\left(\frac{x}{2}\right)^{12} - \frac{14}{165}\left(\frac{x}{2}\right)^{10} + \frac{8}{55}\left(\frac{x}{2}\right)^{8} - \frac{4}{33}\left(\frac{x}{2}\right)^{6} + \left[-\frac{8}{495}\left(\frac{x}{2}\right)^{15} - \frac{4}{55}\left(\frac{x}{2}\right)^{13} + \frac{2}{33}\left(\frac{x}{2}\right)^{11} - \frac{1}{11}\left(\frac{x}{2}\right)^{9} + \frac{2}{11}\left(\frac{x}{2}\right)^{5}\right] \sqrt{\pi}\, e^{x^2/4} \left[1 - \mathrm{erf}\left(\frac{x}{2}\right)\right]\right\}. \tag{37}$$

Equations (33)–(36) were analyzed numerically and the upper bounds on the threshold binding parameters shown in Column E of Table I were found.

VI. APPRAISAL OF THE VARIATIONAL CALCULATIONS: CORELESS POTENTIALS

A. Theorems satisfied

The Hall–Post lower bound[14] on the three-boson ground state energy gives a lower bound of $\frac{2}{3}$ for the entries in Column G of Table II; all the entries satisfy this requirement.

Bruch and Sawada[15] proved exact values for the threshold coupling constant of three bosons would yield entries in Column G of Table II which are less than 1. The entries in Column G are upper bounds to the exact values and for these models are considerable improvements on the Bruch–Sawada bound.

The Hall lower bound[16] for the spin-(3/2) fermion trimer relates the ground state energy to the lowest energy state of the two body problem with one unit of angular momentum. It gives a lower bound of $\frac{2}{3}$ for the entries of Column K. Our upper bounds are quite close to this lower bound.

The Hall lower bound[16] for the spin-(1/2) fermion trimer relates the ground state energy to two body ground states of zero and one unit of angular momentum. It gives a lower bound of $\frac{2}{3}$ to the entries of Column H.

B. Conjectures suggested

Our first conjecture is that the spin-(1/2) trimer generally binds before the spin-(3/2) trimer. This is supported by the entries in Table I and by inspection of the rotational states of the equilateral triangle and of three Hooke's law oscillators. The values in Column D are smaller than the Hall lower-bound values K for the threshold of the spin-(3/2) trimer, so the trial function Eqs. (25) and (26) firmly establishes the conjecture for these models.

Our second conjecture is that three identical fermions generally bind before two bind with one unit of angular momentum. It appears to us to be the fermion analogy of the Bruch–Sawada theorem[15] for bosons and is strongly supported by the entries in Columns J and K of Table II. As remarked at the beginning of Sec. III, the fact that the entries of Column K are less than 1 simplifies the determination that the spin-(3/2) trimer is self-bound.

Our results give no guidance on a third point. The threshold for the spin-(1/2) trimer obtained with Eqs. (25) and (26) lies above the threshold for a spin singlet dimer. Since we have obtained an upper bound on the threshold coupling constant and since Hall's lower bound[16] does not exclude the possibility, the true threshold for the self-bound trimer may lie below the dimer threshold; this would not be an Efimov state.[17] It may be that a variational calculation for the spin-(1/2) trimer with an S state would approach the dimer threshold more closely than our P state calculation does, but our plausibility arguments in Sec. III favored the P state. In a variational calculation in S states we would need to compare the trimer energy with the dimer energy. Above the dimer threshold, using the simple exponential dependences of Eqs. (25) and (26) would probably not be adequate since in a variational calculation of the dimer threshold with the trial function

$$\phi(r) = e^{-\alpha r} \tag{38}$$

the threshold coupling constants for the models of Table I are overestimated by 15%–20%.

C. Discussion

When combined with the lower bounds, the upper bounds on the threshold coupling constants for bound trimers obtained with the elementary trial functions Eq. (1), (24), (25), and (31) narrowly bracket the threshold coupling constants. For three bosons, the threshold variational results of Sitenko and Kharchenko[22] for the square well and of Humberston, Hall, and Osborne[23] for the exponential and Yukawa wells, obtained with more complex trial functions, are close to or slightly below our variational values.

With our elementary trial functions for the coreless models, most of the reduction in the variational calculation could be performed analytically. The results show that our method of modifying the boson trial function to satisfy the requirements for fermion trial functions leads to restrictive variational bounds on the fermion trimer energies.

A Jastrow function has been used in variational calculations on the ^{4}He molecular-boson trimer.[3] We now explore the consequences of similar modifications on it to construct trial functions for study of possible ^{3}He molecular-fermion trimers.

VII. LENNARD-JONES TRIMER

There have been no direct variational searches for binding of ^{3}He trimers. Hall's fermion trimer bounds[16] have been used,[3] though, to argue it is unlikely that the ^{3}He trimer is self-bound. In this section, we present the results of variational calculations of the threshold coupling constant for fermion trimers with Lennard-Jones 12–6 pair potentials. The Lennard-Jones 12–6 pair potential with the parameters of deBoer and Michels[24] is a fair representation[25] of the helium pair potential. We thus obtain a quantitative measure of how far in the coupling constant $^3He_3$ is from being self-bound and see that a moderate uncertainty in the knowledge of the physical coupling constant is not likely to alter our conclusions.

The Lennard-Jones 12–6 pair potential is

$$V(r) = 4\epsilon\left[(\sigma/r)^{12} - (\sigma/r)^{6}\right], \tag{39}$$

and the coupling constant K is

$$K = 4\epsilon m\sigma^2/\hbar^2 . \tag{40}$$

With the deBoer–Michels parameters[24] for ^{3}He, the value of K is 16.6.

We proceed by analogy with the coreless potentials of Secs. IV and V and construct the fermion trimer trial function from a boson trimer trial function used previously[3] in calculations on $^4He_3$. The boson trial function is

$$\Psi_B = \phi(r)\,\phi(s)\,\phi(t), \tag{41}$$

where $\phi(r)$ is the solution of

$$(d^2/dr^2)[r\phi(r)] + (Mm/\hbar^2)[E - V(r)][r\phi(r)] = 0, \tag{42}$$

and M is the variational parameter. This is a simple trial function, but the values obtained with it for the binding of $^4He_3$ have been confirmed by a recent independent calculation.[26]

For the spin-(1/2) trimer we construct the functions ϕ_a and ϕ_s of Eq. (18) by analogy with Eqs. (25) and (26). The function Ψ_B replaces the product of exponentials [Eq. (1)] there.

Similarly for the spin-(3/2) trimer, we replace the product of exponentials [Eq. (1)] in Eq. (32) by Ψ_B.

For both cases the procedure is to choose coupling constants K large enough that there is binding, evaluate the variational ground state energy E_v numerically, and then extrapolate to the case of zero variational energy. The extrapolation can be performed in a way that yields an upper bound on the threshold coupling constant: in a plot of E_v/ϵ against $1/K$, extrapolation of a chord through two points on the curve to zero energy locates an upper bound on the threshold K.[27]

The upper bound on the threshold coupling constant of the spin-(3/2) trimer obtained by the extrapolation is

$$K(3, 3/2) \leq 34.3 . \quad (43)$$

The smallest K value for which binding was found in the variational calculation was 34.4, where $E_v/\epsilon = -7\times 10^{-4}$.

The upper bound on the threshold coupling constant of the spin-(1/2) trimer obtained by the extrapolation is

$$K(3, 1/2) \leq 26.6 . \quad (44)$$

The smallest K value for which binding was found in the variational calculation was 27, where $E_v/\epsilon = -9\times 10^{-4}$.

Our variational energies for the Lennard-Jones 12–6 fermion trimers for several values of the coupling constant K are shown in Table III; these are the data which were used for the extrapolations to obtain Eqs. (43) and (44). They may provide a basis for estimating the binding energy of a near-threshold fermion molecular trimer if such a system is physically realized. Results which may be obtained with more detailed variational calculations could be compared with these values.

TABLE III. Variational energies E_v for the Lennard-Jones 12–6 Fermion trimer as a function of coupling constant K.

	$(-E_v/\epsilon)$[a]	
K[b]	$(s=3/2)$[c]	$(s=1/2)$[d]
40	7.45×10^{-2}	...[e]
38	4.77×10^{-2}	...[e]
36	2.10×10^{-2}	7.49×10^{-2}
35	8.3×10^{-3}	...[e]
34.5	2×10^{-3}	...[e]
34	...[e]	5.37×10^{-2}
32	...[e]	3.38×10^{-2}
30	...[e]	1.65×10^{-2}
28	...[e]	3.5×10^{-3}
27	...[e]	9×10^{-4}

[a]Variational energy E_v scaled with the characteristic energy ϵ of the Lennard-Jones potential Eq. (49).
[b]Coupling constant defined in Eq. (49).
[c]Results for spin-(3/2) trimer using trial function specified in Sec. VII.
[d]Results for spin-(1/2) trimer using trial function specified in Sec. VII.
[e]No calculation performed for this case.

TABLE IV. Threshold coupling constants for Lennard-Jones 12–6 trimers in reduced form.

Ratio	Upper bound[a]
$K(3,0)/K(2,l=0)$	0.939[b,c]
$K(3,1/2)/K(2,l=0)$	1.19[d]
$K(3,1/2)/K(2,l=1)$	0.630[e]
$K(3,3/2)/K(2,l=1)$	0.813[f]

[a]Obtained with the extrapolation of variational energies described in Sec. VII.
[b]Based on an extension of the results of Ref. 3.
[c]Compare with Column G of Table II.
[d]Compare with Column H of Table II.
[e]Compare with column J of Table II.
[f]Compare with Column K of Table II.

We present our results for the threshold coupling constants of the Lennard-Jones trimers in reduced form in Table IV, for comparison with the results for the coreless potentials in Table II. In addition to the fermion trimer results, Eqs. (43) and (44), we use a value of 21.0 for an upper bound on the threshold of the spin-zero boson trimer, $K(3, 0)$. That value is based on a slight extension of the prior three-boson calculations[3] and an extrapolation to zero binding as in the fermion cases here.[27] In scaling the trimer coupling constants we use the threshold coupling constant for a dimer of zero angular momentum[3]

$$K(2, l=0) = 22.362 \quad (45)$$

and for a dimer of one unit of angular momentum[3]

$$K(2, l=1) = 42.4 . \quad (46)$$

For the spin-(3/2) trimer, Hall's lower bound[16] on $K(3, 3/2)$ is (2/3)(42.2) or 28.1. Thus we concluded previously[3] that the spin-(3/2) trimer of ^{3}He is not self-bound. The ratios for the spin-(3/2) trimer threshold and the boson trimer threshold in Table IV are a little larger than for the coreless potentials in Table II.

For the spin-(1/2) trimer, Hall's lower bound[16] on $K(3, 1/2)$ is (2/3)(22.362) or 14.9, which is not strong enough to exclude binding of the spin-1/2 ^{3}He trimer. Our variational result, Eq. (44), is far from the lower bound and from the ^{3}He value of K and unless our trial function is seriously inadequate, the spin-1/2 ^{3}He trimer is not self-bound. We find that the spin-(1/2) trimer threshold is much closer to the singlet dimer threshold for the Lennard-Jones case, Table IV, than for the coreless potentials, Table II.

As with all variational calculations, our results could be superseded by lower values obtained by the use of other trial functions. We believe our Lennard-Jones threshold coupling constants are unlikely to be shifted by more than 20% in such a calculation. The conclusion would remain that there are no bound ^{3}He trimers.

VIII. DISCUSSION

We have shown that a combination of variational calculations using elementary trial functions and lower bound estimates on ground state energies can locate threshold coupling constants for trimer self-binding to within narrow ranges.

Our calculations are for three identical particles interacting via spin-independent central pair potentials. The three-boson threshold calculations are for a state of zero spatial angular momentum and the three-fermion threshold calculations are for a state of one unit of spatial angular momentum. It is notable that our variational estimates for the spin-(1/2) threshold are appreciably above the threshold for a spin-singlet dimer in the same pair potentials.

The ^{3}He trimer is unlikely to be self-bound. If our variational bound for the spin-(1/2) trimer threshold in the Lennard-Jones 12–6 potential is close to the exact value, the physical coupling constant of ^{3}He is far from the threshold. We believe this also leaves it unlikely that the ^{3}He tetramer is self-bound.

It remains an open question what the smallest self-bound cluster of ^{3}He is.

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APPENDIX A: THE RIGID EQUILATERAL TRIANGLE

The wavefunction for three particles in a rigid equilateral triangle configuration provides guidance for the more general case and can be constructed systematically using the group of covering operations on the triangle.[20]

As explicit representations of the exchange operations, we use for P_{12} a rotation about the body-y axis

$$P_{12}=D^l_{mm'}(0,-\pi,0)=(-1)^{l+m}\delta_{-mm'}\ , \tag{A1}$$

and C_{123} is a rotation by $2\pi/3$ about the body-z axis.

$$C_{123}=D^l_{mm'}(-2\pi/3,0,0)=\exp(im2\pi/3)\,\delta_{mm'}\ . \tag{A2}$$

I. Spin-(3/2) trimer

Applying P_{12} from Eq. (A1) on ϕ in Eq. (17) with $l=1$, we see that

$$g^1_1=-g^1_{-1}\ . \tag{A3}$$

Applying C_{123} from Eq. (A2) on ϕ in Eq. (17) we get

$$g^1_1\exp(i2\pi/3)=-g^1_{-1}\ . \tag{A4}$$

Together Eqs. (A3) and (A4) give

$$g^1_1=g^1_{-1}=0\ ,$$

with the result that the $l=1$ state is

$$\phi^1_m=g^1_0D^1_{m0}(\alpha,\beta,\gamma)\ . \tag{A5}$$

II. Spin-(1/2) trimer

Applying P_{12} from (A1) on ϕ_a in Eq. (23),

$$P_{12}b_1=-b_{-1}\ ,\quad P_{12}b_0=b_0\ ,\quad P_{12}b_{-1}=-b_1\ , \tag{A6}$$

and likewise on ϕ_s in Eq. (23),

$$P_{12}a_1=a_{-1}\ ,\quad P_{12}a_0=-a_0\ ,\quad P_{12}a_{-1}=a_1\ . \tag{A7}$$

P_{23} and C_{123} on ϕ_a and ϕ_s, treated similarly, give a set of relations that, combined with (A6) and (A7) and the group relation

$$P_{12}P_{23}=C_{123}\ , \tag{A8}$$

allow us to conclude that

$$b_1=-ia_1\ ,\quad a_0=b_0=0\ ,\quad b_{-1}=ia_{-1}\ . \tag{A9}$$

Use of Eq. (A9) in Eq. (21) gives for the $l=1$ wavefunction

$$\phi_a=(-ia_1)D^1_{m1}+(ia_{-1})D^1_{m-1}\ ,\quad \phi_s=a_1D^1_{m1}+a_{-1}D^1_{m-1}\ . \tag{A10}$$

The rigid equilateral triangle has no internal degrees of freedom; Eqs. (A5) and (A10) constitute wavefunctions of the three-particle system in which the antisymmetry requirements are satisfied by the angular momentum wavefunctions. The rotational energies are, for particles of mass m and triangle side length L: for the spin-(1/2) trimer, $3\hbar^2/2mL^2$; and for the spin-(3/2) trimer, $2\hbar^2/mL^2$. That is, the ground state energy is shifted from the boson ground state[8] by terms in $\hbar^2$ and the spin-(1/2) trimer has lower energy than the spin-(3/2) trimer.

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