Threshold coupling constant for self-binding in a many-boson system*

L. W. Bruch
Department of Physics, University of Wisconsin, Madison, Wisconsin 53706
(Received 20 October 1975)

A sufficient condition for self-binding in a many-boson system interacting via pair potentials is that the coupling constant be greater than the value for which the two-body scattering length first becomes zero. This result is derived and is applied in a discussion of calculations with Lennard-Jones and Morse potential models.

I. INTRODUCTION

A many-boson system interacting via pair potentials can be self-bound for coupling constants appreciably less than those necessary for the existence of bound dimers or trimers. The purpose of this paper is to present an upper bound on the threshold coupling constant for self-binding in a many-boson system with pair potentials; the bound is the coupling constant for which the two-body scattering length first becomes zero.

The proof is based on the use of a cluster expansion of the Rayleigh-Ritz expectation value for the many-boson ground-state energy[1,2] with a Jastrow trial function. In this formulation the criterion[2] for the onset of the self-bound system is that the lead term in the density expansion becomes negative. The lead term is minimized by optimizing the choice of the pair factor in the Jastrow trial function; for coupling constants less than the threshold for a bound dimer, this shows the lead term to be proportional to the scattering length and thus the result follows.

Formally, this method is closely related to considerations of many previous workers.[1-3] Sawada[4] obtained this threshold result by variational methods also; the proof here is a rederivation of his result which apparently is close to the unpublished derivation of Penrose, cited by Sawada. With this result, the threshold coupling obtained by Miller, Nosanow, and Parish[2] for a boson system with Lennard-Jones 12-6 pair potentials is easily recovered and refined. Also, the self-binding of the electron-spin-aligned tritium system found by Etters, Dugan, and Palmer[5] for a Morse-potential model is confirmed.

The bound on the threshold coupling constant is derived in Sec. II; the applications to the Lennard-Jones 12-6 and Morse potential models are contained in Sec. III; an appendix is included which shows the relation of the many-boson threshold calculations to two-body threshold calculations.

II. BOUND ON THRESHOLD COUPLING CONSTANT

Consider a many-boson system in three dimensions, with the Hamiltonian

$$H_N = \sum_{i=1}^{N} \frac{P_i^2}{2m} + \sum_{1\le i<j\le N} \phi(|\vec{r}_{ij}|) \,. \tag{1}$$

The definitions of the coupling constants for the Lennard-Jones and Morse potential models are given in Sec. III; in the discussion of the variation of the coupling constant, what is visualized is that the (central) pair potential has a two-parameter form

$$\phi(|\vec{r}|) = \epsilon\Phi(r/\sigma) \,. \tag{2}$$

The coupling constant K has the following proportionalities:

$$K \propto m\epsilon\sigma^2/\hbar^2 \,; \tag{3}$$

$\hbar$ is the reduced Planck constant.

An upper bound $E_t(N)$ on the ground-state energy $E_0(N)$ is obtained by use of the Jastrow trial function[1]

$$\Psi_J(1, \ldots, N) = \prod_{1\le i<j\le N} f(r_{ij}) \tag{4}$$

in the Rayleigh-Ritz expectation value:

$$E_0(N) \le E_t(N) = \frac{(\Psi_J, H_N\Psi_J)}{(\Psi_J, \Psi_J)} = \sum_{1\le i<j<N} \left[\int d1\cdots dN |\Psi_J|^2 \left(\phi(r_{ij}) + \frac{\hbar^2}{m}(-\tfrac{1}{2})\nabla^2 \ln f(r_{ij})\right)\right] \left(\int d1\cdots dN |\Psi_J|^2\right)^{-1} . \tag{5}$$

Because the ground-state wave function of this many-boson system is non-negative,[6] there is a constraint on the pair factor f,

$$f(r) \ge 0 \,. \tag{4a}$$

Furthermore, to apply cluster expansion methods[1,2]

to the evaluation of Eq. (5), a cluster constraint for f is imposed:

$$\int d\vec{r}\,|f^2(r)-1|<\infty\ . \tag{4b}$$

With the constraint Eq. (4b), in the thermodynamic limit of large particle number N at fixed number density ρ there is a convergent expansion[7] of Eq. (5), in powers of the density, at low density,

$$E_0(N)/N \leq E_t(N)/N = \rho B + O(\rho^2)\ ; \tag{6}$$

the initial slope B is

$$B=\frac{1}{2}\int d\vec{r}\left(\phi f^2+\frac{\hbar^2}{m}|\nabla f|^2\right). \tag{7}$$

A consequence of the convergence statement is that at sufficiently low density the leading term on the right-hand side of Eq. (6) is an accurate evaluation of $E_t(N)/N$, so that if B is negative $E_t(N)$ is negative and the system has lower energy than at zero density.[8]

A sufficient condition for the existence of self-binding is that B is negative. B can be minimized by variation of the pair factor f subject to Eqs. (4a) and (4b). Without the constraints the variation leads to a zero-energy Schrödinger equation for f,

$$-(\hbar^2/m)\nabla^2 f+\phi f=0\ , \tag{8}$$

with a large-r solution in terms of the scattering length a for finite-range potentials or potentials with a van der Waals tail $(1/r^6)$,

$$f\simeq 1-a/r, \quad r\to\infty\ . \tag{9}$$

For zero scattering length, use of Eq. (8) in Eq. (7) shows that B vanishes, the threshold for self-binding.

For nonzero scattering length, Eqs. (8) and (9) as they stand do not yield a function satisfying Eq. (4b). However, this can be immediately remedied for finite-range potentials, which vanish beyond a separation R_0. Modify Eq. (8) by inclusion of a δ-function term[9] at location R larger than R_0,

$$-(\hbar^2/m)\nabla^2 f+\phi f+(\lambda/R^2)\delta(r-R)f=0\ , \tag{10}$$

with the solution f to satisfy

$$f(r)=1\ , \quad \frac{df}{dr}=0\ , \quad r<R\ . \tag{11}$$

For separations just less than R, f satisfies the scattering-length form

$$f(r)=(1-a/r)/(1-a/R)\ , \tag{12}$$

and the choice of λ to achieve Eq. (11) is

$$\lambda=-(\hbar^2 a/m)/(1-a/R)\ . \tag{13}$$

The resulting value for B is

$$B_R=(2\pi\hbar^2 a/m)/(1-a/R)\ . \tag{14}$$

This goes to a limit independent of R as $R\to\infty$,

$$B=2\pi\hbar^2 a/m\ , \tag{15}$$

although the cluster constraint Eq. (4b) does not go to a finite limit. This argument extends, with more detailed estimates of remainders in Eqs. (9) and (12), to the Morse and Lennard-Jones models. The conclusion of this argument is that at low density the leading term in the energy is proportional to the scattering length, which is also a result in optical-model approximations. The conclusion is limited to potential coupling constants less than the threshold K_2 for dimer binding; above K_2 there is a node in the solution of Eq. (8) or (10) and the non-negativeness constraint, Eq. (4a) is no longer satisfied.

III. APPLICATIONS TO LENNARD-JONES AND MORSE POTENTIALS

A. Lennard-Jones 12-6 potential

The Lennard-Jones 12-6 potential

$$\phi(r)=4\epsilon[(\sigma/r)^{12}-(\sigma/r)^6]\ , \tag{16}$$

with coupling constant K,

$$K=4m\epsilon\sigma^2/\hbar^2\ , \tag{17}$$

satisfies Dobrushin's requirements for thermodynamic stability,[10] so that the self-binding obtained for this model is not simply due to collapse at large N.

Miller, Nosanow, and Parish[2] used a pair factor

$$f_{\mathrm{MNP}}(r)=\exp[-\tfrac{1}{2}(b/r)^5] \tag{18a}$$

in a Jastrow trial function, optimized the length b, and obtained a value

$$K_{\mathrm{MNP}}=8.9 \tag{18b}$$

as the threshold for self-binding. Their trial function can be generalized to

$$f_s(r)=\exp[-\tfrac{1}{2}(b/r)^s]\ . \tag{19}$$

With this, the integrals in Eq. (7) reduce to Γ functions,

$$B=(2\pi b^3\epsilon/s)\{4\Gamma(9/s)(\sigma/b)^{12}-4\Gamma(3/s)(\sigma/b)^6 + (s^2/K)\Gamma[2-(1/s)](\sigma/b)^2\}\ . \tag{20}$$

For given s, this is minimized by variation of b and a value K at which $B=0$ is obtained. For $s=5$, the value is 8.78, in good agreement with Eq. (18b). The minimum K obtained by variation of s after the b variation is 8.676, for $s\simeq 4.41$.

The threshold K bound obtained from the condition of zero scattering length is

$$K_J=8.6725\ , \tag{21}$$

only slightly smaller than the value obtained with Eq. (19). For comparison the values of K for the bound dimer[11] K_2 and bound trimer[12] K_3 are known to satisfy

$$K_2 = 22.361 \pm 0.001\,, \quad 14.90 \leq K_3 \leq 21.20\,. \tag{22}$$

B. Morse potential

The Morse potential is

$$\phi(r) = \epsilon(\exp\{2c[1-(r/r_{\min})]\} - 2\exp\{c[1-(r/r_{\min})]\})\,, \tag{23}$$

with coupling constant K,

$$K = m\epsilon r_{\min}^2/\hbar^2 c^2\,. \tag{24}$$

If corrections arising from the finiteness of the potential at $r=0$ are neglected,[13] the threshold coupling constant K_2 for the bound dimer is

$$K_2 = 0.25 \tag{25}$$

and the scattering length is

$$a/r_{\min} = c + \ln(2\sqrt{K}) + \psi(\tfrac{1}{2} - \sqrt{K})\,, \tag{26}$$

where ψ is the digamma function

Etters, Dugan, and Palmer[5] fitted a Morse potential with

$$\epsilon/k_B = 6.19K, \quad r_{\min} = 4.1527\ \text{Å}, \quad \text{and } c = 6.0458 \tag{27}$$

to the calculations by Kolos and Wolniewicz[14] of the electron-spin-triplet potential between two hydrogen atoms. The threshold coupling constant K for boson self-binding obtained from Eq. (26), with $c = 6.0458$, is $K_J = 0.0963$. The value of K for hydrogen with the parameters in Eq. (27) is $K_H \simeq 0.06$, so the criterion for self-binding is not fulfilled for spin-aligned hydrogen; it is fulfilled for spin-aligned tritium, as was found by Etters *et al.*[5,15]

Note added in proof. The situation in two dimensions is a little different, since there the two-body relative motion wave function at the first zero-energy bound state has the cluster property. The threshold coupling constant for the Lennard-Jones 12-6 potential in two dimensions obtained with Eq. (19) is 14.8 for many-boson self-binding and is 20.8 for many-fermion self-binding. These values are consistent with a calculation for two-dimensional helium which found self-binding for ^{4}He but not for ^{3}He [A. D. Novaco and C. E. Campbell, Phys. Rev. B 11, 2525 (1975)].

ACKNOWLEDGMENT

The author thanks Professor C. J. Goebel for helpful discussions.

APPENDIX: RELATION TO TWO-BODY THRESHOLD COUPLING CALCULATIONS

For the two-body calculation with a trial wave function ψ the variational upper bound on the ground-state energy is

$$E_t(2) = \left[\int d\vec{\mathbf{r}}\left(\phi\psi^2 + \frac{\hbar^2}{m}|\nabla\psi|^2\right)\right]\left(\int d\vec{\mathbf{r}}\,\psi^2\right)^{-1}\,. \tag{A1}$$

The numerator in Eq. (A1) is formally the same as B in Eq. (7), and an upper bound on the threshold coupling constant for the dimer is the value when the numerator in Eq. (A1) changes from positive to negative. Kihara, Midzuno, and Shizume[16] obtained such a bound ($K_2 \leq 22.368$ is the value calculated by McGee, following their method) with

$$\psi_t = \exp[-\tfrac{1}{2}(b/r)^s]/r\,. \tag{A2}$$

The trial function in Eq. (19) is not admissible here; the trial function is to be square integrable. The numerator in Eq. (A1) is continuous and finite under the limit ϵ goes to zero of

$$\psi_{t,\epsilon} = \exp[-\tfrac{1}{2}(b/r)^s - \epsilon r]/r \tag{A3}$$

but not of a trial function based on Eq. (19),

$$f_{t,\epsilon} = \exp[-\tfrac{1}{2}(b/r)^s - \epsilon r]\,. \tag{A4}$$

Correspondingly, while the trial function Eq. (19) satisfies the cluster constraint Eq. (4b), the trial function Eq. (A2) does not.

---

*Supported in part by the NSF under grant No. DMR-7419826.

[1]R. Jastrow, Phys. Rev. 98, 1479 (1955).

[2]M. D. Miller, L. H. Nosanow, and L. J. Parish, Phys. Rev. Lett. 35, 581 (1975).

[3]F. Iwamoto, Prog. Theor. Phys. 19, 595 (1958); R. Abe, *ibid.* 19, 713 (1958); V. R. Pandharipande and H. A. Bethe, Phys. Rev. C 7, 1312 (1973).

[4]K. Sawada, Phys. Rev. 148, 160 (1966).

[5]R. D. Etters, J. V. Dugan, and R. W. Palmer, J. Chem. Phys. 62, 313 (1975).

[6]O. Penrose and L. Onsager, Phys. Rev. 104, 576 (1956).

[7]O. Penrose, J. Math. Phys. 4, 1312 (1963). Penrose uses an additional constraint to exclude collapse of the N-particle ground state. This is automatically satisfied for non-negative potentials and is satisfied by the functions $f(r)$ which occur in Sec. III of the present paper. In general, for completeness the results of the optimization of $f(r)$ should be converted to a fictitious pair potential to confirm that they satisfy this condition.

[8]The translational invariance in the Jastrow trial function, Eq. (4), may not be an accurate reflection of the physical situation at low density, with a drop or droplets present, but the inequality between E_0 and E_t remains true.

[9]Another device with the same results as this calculation with the δ function is to solve Eq. (8) in a spherical box of radius R larger than the range R_0, with the requirement that the function equal 1 at the surface,

and then go to the limit of large R.
[10]D. Ruelle, *Statistical Mechanics* (Benjamin, New York, 1969).
[11]J. Lekner, Mol. Phys. 23, 619 (1972); L. W. Bruch and I. J. McGee (unpublished).
[12]The upper bound on K_3 is Eq. (22) is based on an extrapolation of variational calculations using a convexity property, rather than the (plausible) linear extrapolation to a value 20.2 used by L. W. Bruch and I. J. McGee, J. Chem. Phys. 59, 409 (1973).
[13]D. ter Haar, Phys. Rev. 70, 222 (1946).
[14]W. Kolos and L. Wolniewicz, J. Chem. Phys. 43, 2429 (1965).
[15]A fit of the Kolos and Wolniewicz potential minimum with a Lennard-Jones 12-6 potential, which includes a stronger long-range attraction than the Morse potential, yields a coupling constant for the hydrogen case which is 20% short of the critical value in Eq. (21).
[16]T. Kihara, Y. Midzuno, and T. Shizume, J. Phys. Soc. Jpn. 10, 249 (1955).