Near-threshold behavior of the ground-state binding energies of the few-atom systems of ^{4}He and other bosons in two and three dimensions

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The results of accurate variational calculations for the ground-state binding energies of several N-boson systems in two and three dimensions are reported; the systems specifically considered are small ($N = 2$, 3, 4, and 5) clusters of ^{4}He atoms interacting through pairwise Lennard-Jones potentials. Evidence is found strongly suggesting each set of systems have a common functional relationship linking the binding energies and the De Boer quantum constant near threshold for self-binding. These calculations also confirm the existence of a unique threshold value of the interaction strength for all N-boson systems in $2D$. In addition, the linear relation between the binding energies of helium clusters present in $3D$ holds true in $2D$ as well.

I. INTRODUCTION

The binding energies of the ground states of small clusters of bosons in two dimensions were recently evaluated by Bruch and Tjon,[1] and by Cabral and Bruch.[2] Both studies were motivated, in large part, by available experimental data[3] which indicated that at low temperatures rare-gas adatoms on the surface of exfoliated graphite behave as two-dimensional systems (2D). The immediate revelations from the theoretical investigations included the nonappearance of two special effects which occur in systems of three bosons interacting in three dimensions through pairwise potentials, and strong evidence that pairwise-interacting N-boson systems in two dimensions all have the same strength threshold for self-binding. However, Bruch and his collaborators encountered considerable difficulty in handling the more realistic Lennard-Jones potential. They were restricted to simple separable potentials in their integral-equation calculations and to a one-parameter Jastrow function for their variational method. Bruch *et al.* thus suggested that their work be repeated with more realistic potentials and more accurate methods and that the study be extended to cover four- and five-body clusters. This challenge was partially taken up by Tjon himself and more completely and simultaneously by us. Tjon's integral-equation calculations,[4] in which he used a local two-term Gaussian and Yamaguchi-type separable potentials, reaffirmed the correctness of Bruch's conjecture on the coincidence of two-dimensional strength thresholds. In addition, Tjon discovered that there exists a linear relationship between tetramer and trimer binding energies in two dimensions analogous to that in three dimensions; on that account, he has surmised a binding energy of 0.32 K for the ^{4}He tetramer in two dimensions. The work we report here both complements and supersedes the efforts of Tjon and Bruch. We have computed variationally the ground-state binding energies of $N(=2, 3, 4,$ and 5)-boson systems not only in two dimensions but also in three dimensions. We have used the Lennard-Jones (12–6) potential

$$V(r) = 4\epsilon[(\sigma/r)^{12} - (\sigma/r)^6], \tag{1}$$

with ϵ and σ, the strength and range constants, respectively, having the DeBoer and Michels values chosen by Cabral and Bruch.[2] Our variational calculations were based on the (ATMS) Amalgamation of the Two-nucleon correlation into the Multiple Scattering process and quadratures techniques which we developed originally for use in nuclear physics[5] and subsequently tested in a number of applications in molecular physics.[6] The reduced dimensionality for the work in two dimensions poses no new problems as we shall discuss in Sec. II. Thus the results mentioned in Sec. III can be regarded as the most accurate to date.

II. THE ATMS METHOD AND THE N-BOSON SYSTEM

The Hamiltonian for the ground state of each of the two- and three-dimensional systems (3D) considered can be represented by

$$H = -\frac{\hbar^2}{M}\left[\sum_{(ij)}\left(\frac{\partial^2}{\partial r_{ij}^2} + \frac{n-1}{r_{ij}}\frac{\partial}{\partial r_{ij}}\right) + \sum_{(ijk)}\left(\cos\theta(ijk)\frac{\partial^2}{\partial r_{ij}\partial r_{jk}} + \cos\theta(jki)\frac{\partial^2}{\partial r_{jk}\partial r_{ki}} + \cos\theta(kij)\frac{\partial^2}{\partial r_{ki}\partial r_{ij}}\right)\right] + \sum_{(ij)} V(r_{ij}), \tag{2}$$

where

$$\cos\theta(ijk)=\frac{r_{ij}^2+r_{jk}^2-r_{ki}^2}{2r_{ij}r_{jk}}, \tag{3}$$

where M is the mass of each particle in the cluster, n is the dimensionality of space, r_{ij} is the distance between the ith and jth particles, and $\theta(ijk)$ is the angle formed by the ith, jth and kth particles with the jth particle being the vertex. In the sums, (ij) runs over all particle pairs while (ijk) runs over all combinations of three particles. $V(r)$ is the interparticle potential.

To construct the wave functions of these two- and three-dimensional systems we apply the ATMS method. With it, the wave function of a general few-body system is given by a product of two-body correlation functions through which multiple scattering processes are represented. For the helium molecules, their wave functions are determined by

$$\begin{aligned}
&\Psi=\prod_{(ij)}u(r_{ij}),\\
&u(r)=[\psi(r)/\phi(r)]\chi(r),\\
&\chi(r)=\begin{cases}e^{-r^2/(2N\beta^2)} & (r\le r_c)\\ Ce^{-\alpha r}/r^{1/(N-1)} & (r\ge r_c)\end{cases}\\
&\phi(r)=\begin{cases}e^{-r^2/(4\beta^2)} & (r\le r_c)\\ De^{-\gamma r}/r & (r\ge r_c)\end{cases}\\
&\psi(r)=\phi(r)+\frac{1}{E_0-T}V(r)\psi(r),\\
&T=-\frac{\hbar^2}{M}\left(\frac{\partial^2}{\partial r^2}+\frac{n-1}{r}\frac{\partial}{\partial r}\right),
\end{aligned} \tag{4}$$

where β, E_0, and r_c are variational parameters, N is the number of particles in the system, and C and α (D and γ) are determined by smooth continuity of $\chi(\phi)$ at $r=r_c$. We take r_c to be 1.5 β. This choice, which conveniently reduces the number of variational parameters by one, is motivated by the following consideration: β behaves like a range parameter and it can be expected that asymptotic behavior in the radial functions should have begun at a distance equal to 1.5 times the effective range.

Using the wave functions thus constructed, we calculate the energy expectation value of each system which, from Ritz's variational principle, forms an upper bound on the eigenvalue of the Hamiltonian. The integral we evaluate is

$$I=\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\left(\prod_{i=1}^{N-1}\prod_{k=1}^{n}d\xi_i^{(k)}\right)\Psi(\xi)[H\Psi(\xi)], \tag{5}$$

where the $\xi_i^{(k)}$'s are obtained from an orthogonal transformation of the particle coordinates $x_i^{(k)}$ ($i=1,\ldots,N$; $k=1,\ldots,n$) with the center-of-mass coordinates excluded and Ψ normalized. We take as the transformed coordinates

$$\begin{aligned}
&\xi_i^{(k)}=\left(\frac{i}{i+1}\right)^{1/2}\left(-\frac{x_1^{(k)}+\cdots+x_i^{(k)}}{i}+x_{i+1}^{(k)}\right),\\
&i=1,\ldots,(N-1),\quad k=1,\ldots,n.
\end{aligned} \tag{6}$$

For the four- and five-body systems, the integral in Eq. (5) is changed to the form

$$I=\int_0^1\cdots\int_0^1\left(\prod_{i=1}^{N-1}\prod_{k=1}^{n}d\eta_i^{(k)}\right)F(\eta), \tag{7}$$

through a second transformation of variables

$$\begin{aligned}
&\xi_i^{(k)}=K\tan\pi(\eta_i^{(k)}-\tfrac{1}{2}),\quad i=1,\ldots,(N-1),\\
&k=1,\ldots,n,
\end{aligned} \tag{8}$$

where K is an adjustable parameter, which we vary over a fixed range of values. Then we calculate the integral using the quasirandom-number method which we developed in Ref. 5, the mesh points of the $\eta_i^{(k)}$s being distributed with the use of quasirandom numbers. The convergence of the integral is good and, as discussed in Ref. 6, should yield answers accurate to within 0.5% of the exact values.

For the three-body systems, the integral for the energy expectation value is written in terms of the interparticle coordinates as

$$I=2\pi\int_0^{\infty}\cdots\int_0^{\infty}\left(\prod_{(ij)}r_{ij}dr_{ij}\right)\times W(r_{12},r_{23},r_{31})\Psi[H\Psi], \tag{9}$$

where

$$W(r_{12},r_{23},r_{31})=\tfrac{2}{3}\theta(r_{12},r_{23},r_{31})[-\tfrac{1}{4}(r_{12}^4+r_{23}^4+r_{31}^4)+\tfrac{1}{2}(r_{12}^2r_{23}^2+r_{23}^2r_{31}^2+r_{31}^2r_{12}^2)]^{-1/2}, \tag{10}$$

for two-dimensional particles and as

$$I=8\pi^2\int_0^{\infty}\cdots\int_0^{\infty}\left(\prod_{(ij)}r_{ij}dr_{ij}\right)\theta(r_{12},r_{23},r_{31})\Psi(H\Psi), \tag{11}$$

where $\theta(x,y,z)=1$ when the three lengths x, y, and z form a triangle and zero otherwise for three-dimensional particles. Simpson's rule is used in performing these integrations.

TABLE I. Table of ground-state binding energies for two- and three-dimensional dimers, trimers, tetramers, and pentamers of bosons in units of ϵ. The values in parentheses indicate powers of ten.

		Quantum constant, η									
		0.14	0.15	0.16	0.17	0.18	0.19	0.20	0.21	0.22	0.23	0.24
2D	Dimer	1.68(−2)	1.16(−2)	7.30(−3)	4.60(−3)	2.53(−3)	1.25(−3)	5.20(−4)	1.60(−4)			
	Trimer			2.88(−2)	1.88(−2)	1.19(−2)	6.70(−3)	3.30(−3)	1.30(−3)			
	Tetramer					2.84(−2)	1.82(−2)	1.01(−2)	4.70(−3)	1.90(−3)		
	Pentamer								9.41(−3)	3.26(−3)	1.05(−3)	8.00(−5)
3D	Dimer	9.68(−3)	5.07(−3)	2.07(−3)	4.40(−4)							
	Trimer			2.60(−2)	1.55(−2)	7.00(−3)	1.70(−3)					
	Tetramer					3.90(−2)	2.29(−2)	1.01(−2)	2.10(−3)			
	Pentamer								2.30(−2)	7.60(−3)		

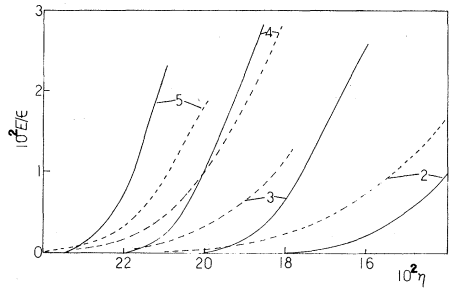

FIG. 1. The ground-state binding energies of few-boson systems interacting through pairwise Lennard-Jones (12, 6) potentials plotted against the constant η. The labeling numerals denote the few-atom systems; the dashed lines are the 2D results, the full curves the 3D. Both sets of lines are drawn through points obtained from the entries on Table I.

III. RESULTS AND DISCUSSION

Table I and Fig. 1 illustrate the general results which we extracted for the ground-state binding energies of four small boson clusters matched against the quantum constant η defined by[7]

$$\eta = \hbar^2/m\epsilon\sigma^2 . \tag{12}$$

The De Boer quantum parameter is $2\pi\eta^{1/2}$. Table II shows the optimum values of the parameters involved in the wave functions and those in the transformation of variables of the four- and five-atom systems. It is worthwhile pointing out that the variation in optimum K values reflects changes in the size of the bosonic systems.

TABLE II. Table of optimum values of the variational parameters for the four- and five-atom systems. 50 000 sampling points were used in the integrals from which these values are derived. The parameter δ is related to E_0 by $E_0 = -\eta\delta^2$.

Four-atom systems		η	β	δ	K
	2D	0.18	2.0	0.20	1.0
		0.19	2.4	0.16	1.2
		0.20	2.4	0.10	1.2
		0.21	3.0	0.08	1.5
		0.22	3.2	0.04	1.5
	3D	0.19	1.4	0.14	1.5
		0.20	1.4	0.10	1.5
		0.21	1.6	0.08	1.7
Five-atom systems					
	2D	0.21	2.8	0.09	1.2
		0.22	3.2	0.06	1.2
		0.23	3.4	0.03	1.5
		0.24	3.8	0.01	1.7
	3D	0.21	1.6	0.16	1.5
		0.22	1.6	0.08	1.5

It is clear for each pair of systems considered that the 2D cluster is more tightly bound near the threshold for self-binding. This is not an artifact of the variational calculations. It has already been shown in the exact numerical calculations of Siddon and Schick[8] that the two-boson system in 2D is bound at a smaller strength constant than in 3D for a given potential. It is also a well-known fact that any attractive square-well potential has at least one bound state in 2D but requires a critical depth for a given range in order to repeat that in 3D.[9] However, as the strength of the interaction increases, the binding energy of each 3D cluster soon overtakes its counterpart in 2D; the point of equality occurs closer and closer to threshold as the number of atoms is increased. It is known[10] that the critical values of η for self-binding in the N-boson system as $N \to \infty$ are η_c^∞ (2D) = 0.271 and η_c^∞ (3D) = 0.461, respectively, so it is obvious that beyond some finite value of N (from the trends indicated in Fig. 1, this is no more than 20), 3D clusters will be bound first and also more strongly at a given value of η. It also appears from Fig. 1 that near threshold the members of each set of clusters exhibit a similar functional relationship between the energy and η. In 2D, the clusters seem to observe the exponential rule first derived by Bagchi[11] for two adatoms, viz.,

$$E_N = C_N \exp[-\beta_N/(\eta_c^N - \eta)], \tag{13}$$

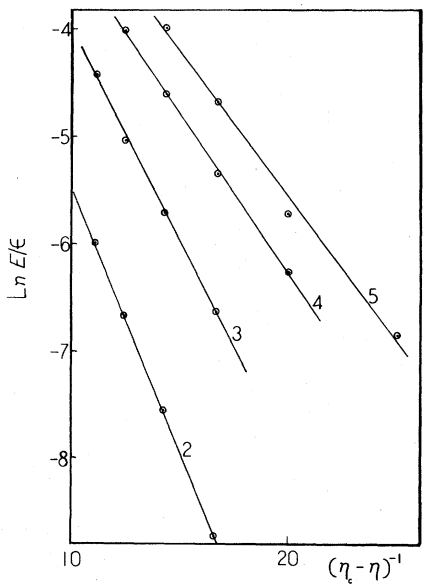

FIG. 2. Plot of the ground-state binding energies of few-boson systems in 2D against η. The functional forms of ordinate and abscissa were selected to expose the exponential relationship between E and η in each system and to confirm the unique value of η_c, here chosen to be 0.271.

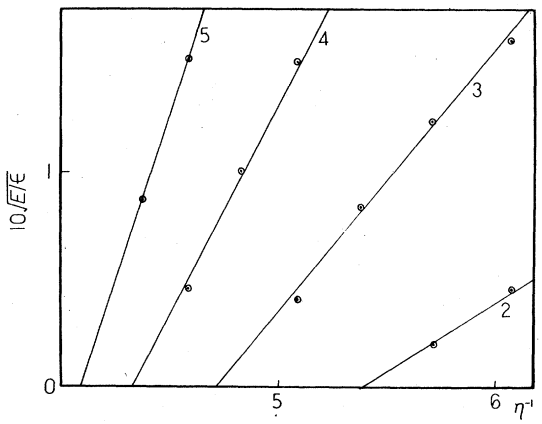

FIG. 3. Plot of the ground-state binding energies of few-boson systems in 3D against η. The functional forms of ordinate and abscissa were selected to reveal the effective-range-theory relation between E and η that is observed by each system.

where C_N and β_N are constants; in 3D, the rule, from effective-range theory, is[12]

$$E_N = K_N(1/\eta_c^N - 1/\eta)^2, \tag{14}$$

with K_N a constant.

To confirm these features as well as Cabral and Bruch's conjecture that $\eta_c^N(2D) = \eta_c^\infty(2D)$ for all N, we have plotted in Fig. 2, $\ln E/\epsilon$ against $(\eta_c - \eta)^{-1}$, taking $\eta_c = 0.271$ for the four clusters in 2D. The unerring linearity of the curves through the points is convincing proof that Eq. (13) and perhaps the Cabral-Bruch hypothesis as well are indeed true. The veracity of Eq. (14) is indicated in Fig. 3 where the threshold behavior for 3D clusters is plotted. In this case the straight lines do not converge on the same point on the abscissa; in 3D, few-boson systems obey the same effective-range

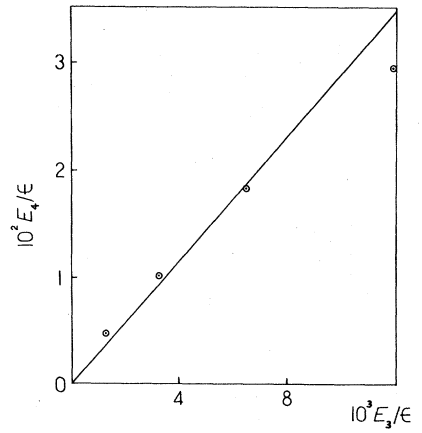

FIG. 4. Plot of E_4 and E_3 for bosons in 2D. The straight line represents the linear relation suggested by Tjon with $E_4/E_3 = 2.9$ (Ref. 4).

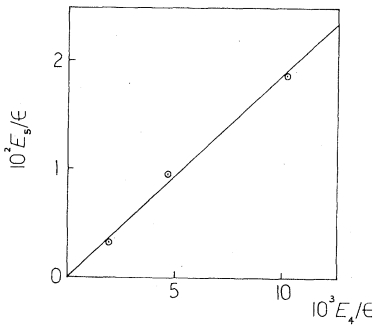

FIG. 5. Plot of E_5 against E_4 for bosons in 2D. The straight line has a slope of 1.9.

relation as for two bosons but they do not possess a common interaction strength for self-binding just to occur. The linear relation between ground-state binding energies of ^{4}He tetramer and trimer observed in 3D (Ref. 6) is also seen to hold here in 2D (see Fig. 4). The single point lying far off the straight line indicates that either the linear relationship breaks down for small values of η or the variational method is inaccurate there. The linear characteristic extends to the pentamer and tetramer binding energies as well (see Fig. 5). We can extract further confirmation of a unique threshold value of η for 2D systems from the passage of both linear curves through the origins of their axes. It can also be surmised that $E_5 \simeq 1.9\ E_4$. We realize that these conclusions are based on variational calculations with the Lennard-Jones potential only. However, in our work on 3D systems of ^{4}He,[6] we have found little difference between the results from various potential forms and thus there is no reason to expect that the present results will be contradicted when other functional forms of the interaction are used.

To conclude, we reiterate that there appears to be a unique value for the threshold strength constant of the pairwise interaction for systems of bosons in 2D. No such uniqueness exists in 3D. The linear relationships between the ground-state binding energies of consecutive clusters of bosons found in 3D are also observed in 2D.

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