PHYSICAL REVIEW A VOLUME 9, NUMBER 2 FEBRUARY 1974

Jastrow-trial-function calculations of trimer ground-state energies*

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(Received 28 September 1973)

Calculations of the trimer ground-state energies of three identical bosons interacting via molecular pair potentials are discussed. The accuracies of variational calculations with a Jastrow trial function and of upper and lower bounds in terms of dimer ground-state energies are determined in a harmonic approximation.

We comment on three points which have arisen in variational calculations of trimer ground-state energies using Jastrow trial functions.[1-5] (i) What accuracy is to be expected of an upper bound on the trimer ground-state energy derived[1] by Bruch and Sawada? (ii) What accuracy is to be expected of a Jastrow trial function[3] for molecular pair potentials with thick cores? (iii) What accuracy is to be expected of the Hall-Post-Stenschke[6,7] lower bound on the trimer ground-state energy? Our discussion is for spinless identical bosons interacting via spherically symmetric pair potentials in three dimensions.

First we consider these points for a molecular system treated in the harmonic approximation. The pair potential $V(r)$ is approximated by a Taylor-series expansion about the potential minimum at $r=R$:

$$V(r) \cong -\epsilon + \tfrac{1}{2} V''(R)(r-R)^2 . \quad (1)$$

There is an important distinction between this situation and the case of Hooke's-law forces with no core, where the potential is

$$V(r) = \tfrac{1}{2} K r^2 . \quad (2)$$

In the case of Eq. (2), it is known[3] that the Jastrow trial function can be adjusted to yield the exact trimer ground-state energy and that this equals[6] the Hall-Post-Stenschke lower bound. The distinction in our treatment is that for Eq. (1) we treat the range of the radial coordinate r, which is 0 to ∞, as being effectively $-\infty$ to ∞. This is valid under the condition that $mR^4V''(R)/\hbar^2$ is much greater than 1 (m is the mass of one particle and $\hbar$ is the reduced Planck constant). This condition is very well satisfied for inert gases heavier than helium. The results of evaluating the two- and three-particle ground-state energies in this approximation are: for the trimer ground-state energy[8] $E_0(3)$,

$$E_0(3) = -3\epsilon + (1+\sqrt{2})(\tfrac{3}{4})^{1/2}\Omega \cong -3\epsilon + 2.091\Omega ; \quad (3)$$

for the Bruch-Sawada upper bound,

$$E_0(3)\,|_{UB} = -3\epsilon + (3/\sqrt{2})\Omega \cong -3\epsilon + 2.121\Omega ; \quad (4)$$

and for the Hall-Post-Stenschke lower bound,[8]

$$E_0(3)\,|_{LB} = -3\epsilon + \sqrt{3}\Omega \cong -3\epsilon + 1.732\Omega , \quad (5)$$

where Ω is defined by

$$\Omega = \hbar[V''(R)/m]^{1/2} . \quad (6)$$

If the Jastrow trial function is written in this approximation as

$$\Psi_J(1,2,3) = \exp[-\alpha(r_{12}-R)^2 - \alpha(r_{13}-R)^2 - \alpha(r_{23}-R)^2] , \quad (7)$$

and the Rayleigh-Ritz expectation value is minimized by variation of α, the trial energy obtained for Eq. (1) is, apart from exponentially small overlap terms, the same as Eq. (4).[9] The parameter α plays the role of the mass parameter M used in a variational calculation for helium by Bruch and McGee; the optimal value corresponds to the use of the two-body reduced mass ($M=1$) in the α in Ψ_J. For Eq. (2), it is known[3] that the optimal value is $\frac{2}{3}$ of the two-body reduced mass ($M=\frac{2}{3}$).

As an example not restricted to the harmonic approximation, we have carried through for a hydrogen trimer $(H_2)_3$ a calculation similar to our helium calculations[2]. A Lennard-Jones 12-6 pair-potential model[10] with characteristic energy $\epsilon = 37.0$ K and length $\sigma = 2.928$ Å was chosen to illustrate the magnitudes; more refined models are available.[11] The trimer ground-state energy then has an upper bound of −10.8 K (Bruch-Sawada) and a lower bound of −20.5 K. The minimum trial energy with the variational wave function of

Ref. 2 is −11.9 K for an M parameter equal to 0.85.

Finally, the calculations reported in the previous paragraph used only a restricted type of Jastrow trial function. For helium, the results of recent variational calculations have raised the question of whether this trial function misses much of the ground-state energy so that the lower bound may give an accurate indication of the trimer ground-state energy in this extremely anharmonic case. One of the recent calculations, by Lim,[5] can be shown to be in error.[12] The other, by Bosanac and Murrell,[4] is a multiparameter calculation of some complexity. We believe the accuracy of the lower bound for helium trimers is an open question, which may be settled by further multiparameter calculations.

We thank Professor J. N. Murrell and Professor T. K. Lim for sending preprints of their papers.

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*Work supported in part by the National Science Foundation, through the U. S.-Japan Cooperative Science Program, and in part by the National Research Council of Canada.

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[12]One method is to observe that in bringing the Morse potential he treated to a form fitted to the trial function he used, Lim (Ref. 5) effectively introduced a hard core in the pair potential at 2.4 Å. If the evaluation of the lower bound is repeated with the Morse pair potential containing the 2.4-Å core, the lower-bound excludes a bound trimer.