The equivalent two-body and delta energy lower bounds for N-boson systems

1989 J. Phys. A: Math. Gen. 22 179

(http://iopscience.iop.org/0305-4470/22/2/007)

J. Phys. A: Math. Gen. 22 (1989) 179–183. Printed in the UK

The equivalent two-body and delta energy lower bounds for N-boson systems

Richard L Hall

Department of Mathematics, Concordia University, 1455 de Maisonneuve Blvd W, Montreal, Quebec, Canada H3G 1M8

Received 7 June 1988, in final form 1 September 1988

Abstract. We study the ground-state energy of a system of N identical bosons, each having mass m, which interact in one dimension via the pair potential $V(x) = \gamma f(x/a)$ and obey non-relativistic quantum mechanics. A recent energy lower bound based on the known exact solution for the delta potential is compared to an earlier bound provided by the equivalent two-body method. The delta bound is good whenever the potential is very narrow and deep. For any bounded potential, the earlier energy bound is always better for large N. Detailed results and graphs are given for the sech-squared potential and the square-well potential.

1. Introduction

We consider a system of N identical bosons which interact in one spatial dimension via central pair potentials and obey non-relativistic quantum mechanics. The Hamiltonian for the N-particle system (with the kinetic energy of the centre of mass removed) is given explicitly by

$$H = \frac{1}{2m}\sum_{i=1}^{N} p_i^2 - \frac{1}{2Nm}\left(\sum_{i=1}^{N} p_i\right)^2 + \sum_{\substack{i,j=1\\ i<j}}^{N} \gamma f(x_{ij}/a) \tag{1.1}$$

where m is the mass of a particle, $x_{ij} = |x_i - x_j|$ is a pair distance, $f(x)$ is the potential shape, a is a length parameter and γ is the coupling constant. The purpose of the present paper is to compare two general energy lower-bound formulae for estimating the ground-state energy of E of H. The first method (Hall and Post 1967) relates E to the energy of a specially constructed two-particle problem; the second method (Perez *et al* 1988) relates E to the energy of a corresponding N-boson system in which the particles interact via a delta potential which has a specially chosen coupling constant.

We shall first express both of the energy bounds in terms of two convenient energy and coupling parameters, and then we shall apply these bounds to the sech-squared potential and to the square-well potential for which all the details of the two approximations can be worked out exactly.

2. The energy bounds

We define the following dimensionless energy and coupling parameters which we shall

0305-4470/89/020179+05$02.50

use to express all the N-body energy results in this paper:

$$\mathscr{E} = \frac{mEa^2}{\hbar^2(N-1)} \qquad v = \frac{m\gamma a^2 N}{2\hbar^2}. \tag{2.1}$$

It is explained in Hall and Post (1967) that a remarkable consequence of the permutation symmetry of boson states is that the energy E of the N-body Hamiltonian H may be closely estimated by considering the energy of a one-particle (or reduced two-particle) Hamiltonian $\mathbb{H}$ given by

$$\mathbb{H} = -\mathrm{d}^2/\mathrm{d}x^2 + vf(x) \tag{2.2}$$

where v is defined by (2.1). If, for a given value of v, $L(v)$ denotes the bottom of the spectrum of $\mathbb{H}$ and $U(v)$ is the lowest variational estimate of $\mathbb{H}$ by means of Gaussian wavefunctions $\phi(x) = \exp(-\alpha x^2)$, then we have

$$\inf_{\psi} \frac{(\psi, \mathbb{H}\psi)}{(\psi, \psi)} = L(v) \leqslant \mathscr{E} \leqslant U(v) = \min_{\alpha} \frac{(\phi, \mathbb{H}\phi)}{(\phi, \phi)}. \tag{2.3}$$

In the case of the harmonic oscillator with shape $f(x) = x^2$ we immediately recover from (2.3) the following well known exact expression for the N-boson energy:

$$f(x) = x^2 \qquad L(v) = \mathscr{E} = v^{1/2} = U(v). \tag{2.4}$$

In the case of the delta potential $f(x) = -\delta(x)$ we have shown (Hall 1967a) that $L(v) = -\frac{1}{4}v^2$, and $U(v) = -v^2/2\pi$. Meanwhile, McGuire (1964) has found the exact solution to the N-boson problem in which the pair potential is $V(x) = -\gamma\delta(x/a) = -\gamma a\delta(x)$, and we therefore know from this work that the N-body energy is given by the formula:

$$E = -N(N^2-1)(\gamma a)^2 m/24\hbar^2. \tag{2.5}$$

Consequently, in terms of the parameters (2.1), we may write for this problem:

$$f(x) = -\delta(x) \qquad L(v) = -\tfrac{1}{4}v^2 \leqslant \mathscr{E} = -\tfrac{1}{6}v^2(1+1/N) \leqslant U(v) = -v^2/2\pi. \tag{2.6}$$

Hence, the lower bound, which of course is exact for $N = 2$, gradually weakens as N increases; for very large values of N, the lower bound is 50% below the exact value. For very narrow and deep potentials, such as the delta potential, the lower bound described below will usually be more appropriate.

Perez *et al* (1988) have used the exact solution (2.1) of the N-boson problem with delta potentials to extend the one-particle result of Spruch (1961) to many particles. They obtain the following very simple formula for a lower bound:

$$E \geqslant -N(N^2-1)I^2 m/24\hbar^2 \tag{2.7}$$

in which the factor $(\gamma a)^2$ in McGuire's (1964) delta formula (2.5) has been replaced by I^2, where the integral I is given by

$$I = \int_{-\infty}^{\infty} |V_-(x)|\,\mathrm{d}x = \gamma a \int_{-\infty}^{\infty} |f_-(t)|\,\mathrm{d}t \qquad t = x/a \tag{2.8}$$

and $V_-(x) = V(x)$ when $V(x)$ is negative but is zero when $V(x)$ is positive (and similarly for the shape function $f(x)$). If we now express this result in terms of our dimensionless parameters (2.1) we obtain the following lower-bound formula:

$$\mathscr{E} \geqslant D_N(v) = -\tfrac{1}{6}v^2(1+1/N)J^2 \qquad J = \int_{-\infty}^{\infty} |f_-(t)|\,\mathrm{d}t \qquad N \geqslant 2. \tag{2.9}$$

In the case that the pair potential has the shape $f(x) = -\delta(x)$, then $J = 1$ and the lower bound (2.9) is equal to the exact energy given in (2.6). Our task is now to compare (2.3) with (2.9) for some more interesting examples.

3. The sech-squared potential

The sech-squared potential is discussed in Flügge (1974) and has the shape

$$f(x) = -\mathrm{sech}^2(x). \tag{3.1}$$

The lowest eigenvalue of the corresponding one-particle Hamiltonian $\mathbb{H}$ which, by (2.3), yields a lower energy bound to $\mathscr{E}$, is given by the formula

$$\mathscr{E} \geqslant L(v) = -[(v+\tfrac{1}{4})^{1/2} - \tfrac{1}{2}]^2. \tag{3.2}$$

Meanwhile, the integral J of (2.9) becomes, in this case,

$$J = \int_{-\infty}^{\infty} |f_-(t)|\,\mathrm{d}t = \int_{-\infty}^{\infty} \mathrm{sech}^2(t)\,\mathrm{d}t = 2. \tag{3.3}$$

Consequently, the lower bound given by (2.9) for this example is

$$\mathscr{E} \geqslant D_N(v) = -\tfrac{2}{3}v^2(1+1/N) \qquad N \geqslant 2. \tag{3.4}$$

If the product γa of the coupling and the range is kept constant, and a is made small, then we see that $\mathscr{E}$ and v^2 vanish together (each like a^2). In this limit, one can show, by using Taylor's theorem, that $L(v) \approx D_2(v) = -v^2$; consequently, for $N > 2$, in this region, $D_N(v)$ will be above $L(v)$, i.e. it will be a better lower bound to $\mathscr{E}$. Graphs of $L(v)$, $D_2(v)$, and $D_\infty(v)$ for small v are shown in figure 1. For $v > 0.3$, however, $L(v)$ is a better lower bound for all values of γ and a and for all $N \geqslant 2$. If one considers a given potential (so that γ and a are fixed), then v increases with N and, for a large system, $L(v) \approx -v$. Since $\mathscr{E}$ is proportional to $E/(N-1)$, this indicates that the binding energy increases like N^2 (as indeed it does) rather than like N^3, as the $D_N(v)$ lower bound (3.4) would suggest.

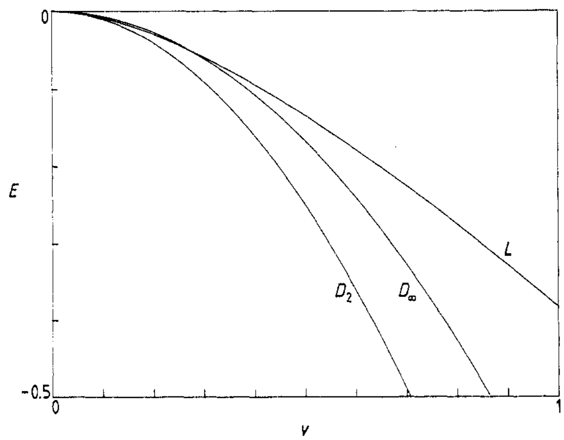

Figure 1. The lower energy bounds $L(v)$, $D_2(v)$ and $D_\infty(v)$ for the N-boson problem in one dimension with the sech-squared pair potential. For $v > 0.3$, $L(v)$ is always above $D_N(v)$, $N \geqslant 2$.

4. The square-well potential

The shape function for the square-well potential is given by

$$f(x)=\begin{cases}-1 & |x|<1 \\ 0 & |x|\geqslant 1.\end{cases} \tag{4.1}$$

The bottom of the spectrum $L(v)$ of $\mathbb{H}$ for this problem and the best upper estimate $U(v)$ via a Gaussian wavefunction are given (Hall 1967a) in parametric form by the following equations:

$$\begin{aligned} &L(v)=-t^2\tan^2 t \qquad t\in[0,\pi/2) \\ &v=t^2/\cos^2 t \end{aligned} \tag{4.2}$$

$$\begin{aligned} &v=\tfrac{1}{2}\sqrt{\pi}\,t\,\mathrm{e}^{t^2} \qquad t\in[0,\infty) \\ &U(v)=-v\,\mathrm{erf}(t)+\tfrac{1}{2}t^2 \qquad \mathrm{erf}(t)=\frac{2}{\sqrt{\pi}}\int_0^t \mathrm{e}^{-\xi^2}\,\mathrm{d}\xi. \end{aligned} \tag{4.3}$$

The integral J required in the delta lower bound (2.9) has the value $J=2$ for the potential (4.1). Therefore the lower energy bound (2.9) becomes, in this case, exactly the same as for the sech-squared potential, namely

$$\mathscr{E}\geqslant D_N(v)=-\tfrac{2}{3}v^2(1+1/N) \qquad N\geqslant 2. \tag{4.4}$$

The situation here is rather similar to that for the sech-squared potential. The results for small v are shown in figure 2. Since we now include the upper bound $U(v)$, it is particularly clear that, for large v, $L(v)$ is close to $U(v)$ and therefore also to the unknown exact energy $\mathscr{E}$; the lower bound $L(v)$ is better than $D_N(v)$, for all $N\geqslant 2$, whenever the parameter values are such that $v>0.4$; for large v, $L(v)\simeq -v$ whereas $D_N(v)\simeq -\tfrac{2}{3}v^2$.

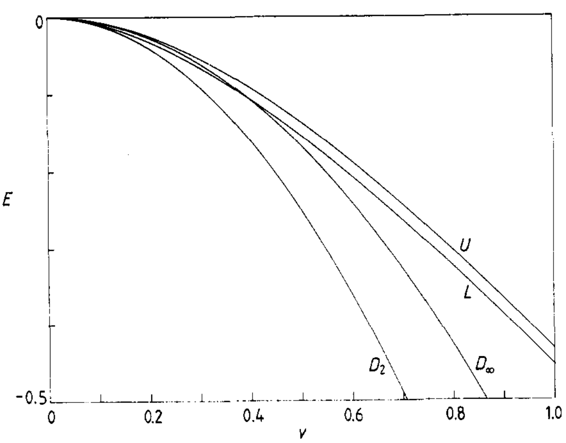

Figure 2. The lower energy bounds $L(v)$, $D_2(v)$ and $D_\infty(v)$, and the upper bound $U(v)$, for the N-boson problem in one dimension with the square-well pair potential. For $v>0.4$, $L(v)$ is always above $D_N(v)$, $N\geqslant 2$.

5. Conclusion

The delta lower bound (2.9) given by Perez *et al* (1988) is effective for any attractive potential in one spatial dimension which closely approximates a delta potential. In other cases the bound is likely to be weak. For any given potential, the delta lower bound always varies for large N approximately as N^3. If the boson delta lower bound can somehow be extended to the three-dimensional case, then the result would probably improve the known energy lower bound for the gravitational boson problem in which the potential shape is $f(r)=-1/r$ and for which the three-dimensional version of (2.3) yields $-v^2/4 \leqslant \mathscr{E} \leqslant -2v^2/3\pi$ (Post 1962). However, without some suitable modification to the singularity, the attractive delta potential in three spatial dimensions leads to infinite binding energy even for just two particles (Hall 1967a). The variational upper bound alone can certainly be sharpened (Hall 1988).

In one dimension progress has been made in exploiting the exact delta-potential results for N-fermion systems (Yang 1968, Lieb and de Llano 1978). Meanwhile an 'equivalent two-body' lower bound for N-fermion systems (in any number of dimensions) has also been devised (Hall 1967b, 1979).

Acknowledgments

The author would like to thank the Natural Sciences and Engineering Research Council of Canada for partial financial support of this work under grant number A3438.

References

Flügge S 1974 *Practical Quantum Mechanics* (Berlin: Springer)
Hall R L 1967a *Proc. Phys. Soc.* **91** 787
—— 1967b *Proc. Phys. Soc.* **91** 16
—— 1979 *Phys. Rev.* C **20** 1155
—— 1988 *J. Math. Phys.* **29** 990
Hall R L and Post H R 1967 *Proc. Phys. Soc.* **90** 381
Lieb E H and Llano M 1978 *J. Math. Phys.* **19** 860
McGuire J B 1964 *J. Math. Phys.* **5** 622
Perez J F, Malta C P and Coutinho F A B 1988 *J. Phys. A: Math. Gen.* **21** 1847
Post H R 1962 *Proc. Phys. Soc.* A **79** 819
Spruch L 1961 *Lectures in Theoretical Physics* vol 4, ed W E Brittin, B W Dows and J Dows (New York: Wiley) p 200
Yang C N 1968 *Phys. Rev.* **168** 1920