

### Energy trajectories for the $N$ -boson problem by the method of potential envelopes

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This paper concerns the ground-state energy  $E_N$  of a system of  $N$  identical bosons interacting via the attractive central pair potential  $V(r_{ij}) = -V_0 f(r_{ij}/a)$  and obeying nonrelativistic quantum mechanics. It is assumed that the potential shape  $f$  is decreasing and can be represented as the envelope of each of two complementary families of power-law potentials  $\alpha + \beta r^p$  (one family is above  $f$  and the other below) for suitable fixed  $p = p_1$  and  $p = p_2$ . If  $\epsilon = -ma^2 E_N / (N - 1)\hbar^2$  and  $v = NmV_0 a^2 / 2\hbar^2$ , then it is proved that the entire collection of nonintersecting energy trajectories  $\epsilon = F_N(v)$ ,  $N = 2, 3, 4, \dots$ , is bounded between the fixed curves  $(v, \epsilon) = (-\gamma(p)[s^3 f'(s)]^{-1}, (v/2)[2f(s) + sf'(s)])$ , where the curve parameter  $s > 0$ , and  $p = p_1, p_2$ . Potentials, for example, with shapes  $f(r) = \alpha_1/r + \alpha_2/(r + \alpha_3) - \alpha_4 \ln r - \alpha_5 \text{sgn}(q)r^q$ , where  $\alpha_i \geq 0$  and  $|q| \leq 1$ , have the  $\gamma$  numbers  $\gamma(-1) = 2$  and  $\gamma(1) = 12/\pi$ . The appropriate  $\gamma$  numbers are provided for other classes of potential shape including perturbed harmonic oscillators, and also for problems in one spatial dimension. The method yields in effect a recipe for the way  $E_N$  depends on  $N$  and all the parameters of the pair potential.

#### I. INTRODUCTION

In this article we shall be concerned with the problem of finding the ground-state energy  $E_N$  of a system composed of  $N$  identical particles interacting by attractive pair potentials. The main emphasis is on systems of bosons although the results apply equally well to the lowest spatially symmetric states of few-fermion systems provided there are enough internal variables (spin, iso-spin, color) to make such states accessible. Our approach is to exploit the boson symmetry to relate the  $N$ -body problem to suitable two-body problems, and to use geometrical methods to analyze this relationship. Geometry is involved because our results hinge on the way the energy varies with the coupling constant, and this leads to the study of families of noninteracting "energy trajectories". We are using the general principle<sup>1</sup> from dynamic programming that in optimization one should try to study families of nearby problems.

We assume a translation-invariant Hamiltonian  $H$  for the  $N$ -particle system with the form

$$H = \sum_{i=1}^N \frac{\vec{p}_i^2}{2m} - \frac{\left(\sum_{i=1}^N \vec{p}_i\right)^2}{2mN} + \sum_{i=1}^N \sum_{i < j} V_{ij},$$

i. e.,

$$H = \sum_{i=1}^N \left[ \frac{(\vec{p}_i - \vec{p}_i)^2}{2mN} + V_{ij} \right], \tag{1.1}$$

where

$$V_{ij} = -V_0 f(r_{ij}/a) \tag{1.2}$$

and  $V_0$  and  $a$  are, respectively, the depth and range parameters of the attractive central potential with shape  $f$ . The complexity of the  $N$ -boson problem is greatly reduced by the necessary per-

mutation symmetry of the wave functions. If  $\Phi(\vec{\rho}_2, \vec{\rho}_3, \dots, \vec{\rho}_N)$  is any normalized boson "trial" function of the  $N - 1$  Jacobi orthogonal relative coordinates,<sup>2</sup>  $\vec{\rho}_2 = (\vec{r}_1 - \vec{r}_2)/\sqrt{2}$ ,  $\vec{\rho}_3 = (\vec{r}_1 + \vec{r}_2 - 2\vec{r}_3)/\sqrt{6}$ , etc., then we have<sup>2</sup>

$$E_N \leq (\Phi, H\Phi) = (\Phi, \mathcal{H}\Phi), \tag{1.3}$$

where the one-particle ("reduced" two-particle) Hamiltonian  $\mathcal{H}$  is given by

$$\mathcal{H} = -(N - 1) \left[ \frac{\hbar^2}{2m} \Delta_{\rho_2} + \frac{N}{2} V_0 f(\sqrt{2} \rho_2/a) \right]. \tag{1.4}$$

Equation (1.3) is fascinating because it suggests that there may be a relationship between  $E_N$  and the eigenvalues  $e_i$  of  $\mathcal{H}$ . The *ad hoc* approximation  $E_N \approx e_0$  was used by Wigner<sup>3</sup> in 1933 at the dawn of contemporary nuclear physics (with  $N = 3$  and 4) and the first rigorous relationship was discovered in 1956 by Post<sup>4</sup> who proved that  $E_N \geq e_0$ , for all  $N \geq 2$ . Subsequent developments<sup>2</sup> in this area of lower-bound theory have led, for example, to bounds suitable for fermion systems and atom-like systems,<sup>5</sup> and also to bounds on the energies of the excited states.<sup>6</sup>

Our present discussion of the  $N$ -boson problem is further simplified by the use of the following dimensionless quantities in which, it should be noted, the sign of the energy has been changed (for large  $N$ , and for nonconfining potentials, the variable  $\epsilon$  is proportional to the binding energy per particle):

$$\begin{aligned} v &= NmV_0 a^2 / 2\hbar^2, \\ \epsilon &= -mE_N a^2 / (N - 1)\hbar^2, \\ \hat{h} &= \Delta_{\vec{x}} + v f(x), \\ \vec{x} &= \sqrt{2} \vec{\rho}_2 / a. \end{aligned} \tag{1.5}$$

If  $\Psi_N$  is the suitably normalized *exact* ground state of the  $N$ -particle system, then we may write from Eqs. (1.3) and (1.5)

$$\epsilon = (\Psi_N, \hat{h}\Psi_N) \equiv F_N(v). \quad (1.6)$$

Thus, for each given potential shape  $f$ , there will be a family  $\{F_N\}$  of  $(v, \epsilon)$  curves or energy trajectories labeled by  $N=2, 3, 4, \dots$ . For the harmonic oscillator we have  $f(x) = -x^2$  and the trajectories all coalesce in this case into the single exact curve  $\epsilon = -3v^{1/2}$ . For the attractive "delta-function" potential<sup>7,8</sup> in *one* spatial dimension  $f(x) = \delta(x)$ , and we have for all  $N \geq 2$

$$\epsilon = F_N(v) = \frac{1}{6} \left( 1 + \frac{1}{N} \right) v^2. \quad (1.7)$$

Although this  $\delta$ -function potential only acts in one dimension and is not smooth as are the potentials we shall principally study in this paper, we exhibit the curves (1.7) in Fig. 1 as an illustration of the geometry of the energy trajectories for an exactly soluble case. Unfortunately, these two examples exhaust the list of exact solutions known for all  $N$ . In general, we can prove by a variational argument (Sec. II) that the energy trajectories  $F_N$  cannot intersect; we can also bound these curves for all  $N \geq 2$  by the following general inequalities:

$$F_2(v) \geq F_N(v) = \epsilon \geq F_g(v), \quad (1.8)$$

where  $F_2$  is the exact solution of the two-body problem, and  $F_g$  (which also does not depend on  $N$ ) is obtained by the use of a Gaussian trial func-

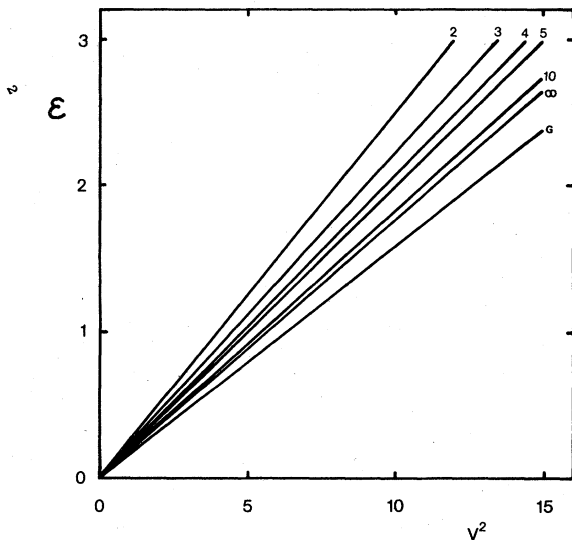


FIG. 1. Exact energy trajectories  $\epsilon = F_N(v)$ , labeled by  $N$ , for the attractive  $\delta$ -function potential in one dimension; and Gaussian trajectory bound  $F_g(v)$ ;  $v = mNV_0 a^2 / 2\hbar^2$  and  $\epsilon = -mE_N a^2 / (N-1)\hbar^2$ .

tion. In many cases the  $N$  dependence of  $E_N$  is largely accounted for by the  $N$  dependence in  $v$  and  $\epsilon$  so that the functions  $F_N$  do not vary strongly with  $N$ .

The equality  $F_2(v) = F_g(v)$  occurs if, and only if,  $f$  corresponds to a harmonic oscillator.<sup>9,10</sup> For short-range potentials the bounds can be very close,<sup>2</sup> and for the linear potential  $f(x) = -x$  which we have recently studied (along with general power-law potentials, see Sec. III) we can determine  $E_N$  in this way with error  $< 0.15\%$ . Mathematically rigorous bounds such as these are *themselves* useful both for the construction of models for few-particle problems and as tests for alternative many-body techniques such as the numerical solution of the Faddeev equations.<sup>11</sup>

However, the main purpose of the present paper is to describe a new geometrical method, which we call the "method of potential envelopes," for determining bounds on the energy trajectories  $F_N$ . We first find in Sec. III the trajectory bounds  $F_2$  and  $F_g$  for the power-law potentials

$$f(x) = -\text{sgn}(p)x^p, \quad p \geq -1. \quad (1.9)$$

We then consider, for a given fixed  $p$ , a potential with decreasing shape  $f$  which may be represented as the envelope of a family  $\{f_s\}$  of power-law potentials given by

$$f_s(x) = \alpha(s) - \beta(s) \text{sgn}(p)x^p, \quad (1.10)$$

where  $s$  is a parameter which labels the curves in the family. Since we know  $F_2$  and  $F_g$  for each of the component potentials  $f_s$ , we can use this information to find trajectory bounds for the potential  $f$  which is the envelope of the  $f_s$ . A sufficient condition for definite energy bounds is that every  $f_s$  must correspond either to a stronger or to a weaker potential than  $f$  itself. For example, the tangents to  $f(x) = e^{-x}$  corresponds to a collection of linear potentials each of which is weaker than the exponential potential. We obtain in this way trajectory bounds  $F_L$  and  $F_U$  (the subscripts refer to "lower" and "upper" in the sense of the energy  $E_N$  which has opposite sign to  $\epsilon$ ) satisfying

$$F_U(v) \leq F_g(v) \leq \epsilon \leq F_2(v) \leq F_L(v). \quad (1.11)$$

The pleasing outcome of this study is that we have been able to find a simple universal formula which gives  $F_U$  and  $F_L$  *directly* in terms of the potential shape  $f$ , namely,

$$F(v) = \frac{1}{2}v[2f(s) + sf'(s)], \quad (1.12)$$

$$v = -\gamma(p)[s^3 f'(s)]^{-1}, \quad s > 0.$$

For each value of  $p$ , we need just two  $\gamma$  numbers,  $\gamma_L(p)$  and  $\gamma_U(p)$ , which respectively determine  $F_L$  and  $F_U$ ; moreover, these numbers turn out to

be precisely the same factors which yield  $F_2$  and  $F_g$  via Eq. (1.12) for the corresponding power-law potential shape  $f(s) = -\text{sgn}(s)s^p$ .

As an illustration, suppose  $p = 2$ , then for the harmonic oscillator with shape  $f(x) = -x^2$  we already know  $F_2(v) = F_N(v) = F_g(v) = -3v^{1/2}$ , and consequently from Eq. (1.12) we have  $\gamma_L(2) = \gamma_U(2) = \frac{9}{2}$ . Now consider the Gauss potential  $e^{-x^2}$  which can certainly be written as the envelope (above) of a family of the form  $\alpha - \beta x^2$ , so that Eq. (1.12) yields  $\epsilon \geq F_U(v) = ve^{-s^2}(1 - s^2)$ ,  $v = 9e^{s^2}/4s^4$ , and  $0 < s \leq 1$ . Without changing  $\gamma$  we can, of course, immediately apply Eq. (1.12) to find  $F_U$  for  $f(x) = e^{-x}$  or  $f(x) = x^{-1} - x$  or for any smooth potential shape which lies above a family of parabolas. Potential shapes with corners can first be approximated by smooth curve curves on the appropriate side, and the formula (1.12) may then be applied to this approximation.

As a further illustration, suppose  $f(x) = x^{-1} - x^q$  for fixed  $q$  in the range  $0 < q \leq 1$ . Such potentials are of interest as nonrelativistic approximations for the central part of the quark-quark interaction<sup>13,14</sup> (since we consider only a one-component Schrödinger equation in the present article our results may be applied directly to  $N$ -quark systems only for  $N \leq 3$ ). In Sec. IV we shall show that  $\gamma_L(-1) = 2$  and  $\gamma_U(1) = 12/\pi$ . This class of potentials has the property that  $f$  lies above its tangents ( $p = 1$ ) of the form  $\alpha + \beta x^{-1}$ . Consequently, the trajectory bounds  $F_U$  and  $F_L$  provided by Eq. (1.12) are "magnifications" of each other for if  $(v, \epsilon)$  is a point of  $F_L$ , then  $(\mu v, \mu \epsilon)$  is a point of  $F_U$ , where  $\mu = 6/\pi$ .

Equation (1.12) is not without some interest even for  $N = 2$  and in view of the usually intractable nature of the many-body problem we expect that the existence of such a general formula, valid for all  $N \geq 2$ , will be of practical importance for exploring the implications of various potential shapes for the  $N$ -boson problem.

II. THE FUNDAMENTAL ENERGY BOUNDS

The lower energy bound is represented in the notation of this paper by the inequality  $F_N(v) \leq F_2(v)$ . By an immediate generalization of the proof of this result in Ref. 2 we now prove that the energy trajectories  $F_N$  do not intersect, i.e.,

$$F_N(v) \leq F_K(v), \quad N > K. \tag{2.1}$$

For this argument it is essential to use Jacobi orthogonal relative coordinates  $\{\vec{\rho}_i\}$  which have the property that  $\vec{\rho}_{n+1}$  is symmetric in the individual-particle coordinates  $(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_n)$ . We suppose that  $\{\Psi_N^i\}$  represents the orthonormal eigenstates corresponding to the energies  $E_N^i \leq E_N^{i+1}$  of the  $N$ -boson problem and we write for fixed  $K$ ,  $2 \leq K < N$ ,

$$\begin{aligned} & \Psi_N^0(\vec{\rho}_2, \vec{\rho}_3, \dots, \vec{\rho}_N) \\ &= \sum_i C_i \Psi_K^i(\vec{\rho}_2, \vec{\rho}_3, \dots, \vec{\rho}_K) G_i(\vec{\rho}_{K+1}, \vec{\rho}_{K+2}, \dots, \vec{\rho}_N), \end{aligned} \tag{2.2}$$

where the  $G_i$  have norm one but are not necessarily orthogonal, and the summation over  $i$  includes, if necessary, integration over the continuum. It follows that

$$\|\Psi_N^0\|^2 = \sum_i |C_i|^2 = 1, \tag{2.3}$$

and from Eq. (1.6) we have

$$\epsilon = (\Psi_N^0, \hat{h}\Psi_N^0) = \sum_i |C_i|^2 (\Psi_K^i, \hat{h}\Psi_K^i). \tag{2.4}$$

Now, for a given fixed value of  $v$  (the product  $V_0\alpha^2$  must be adjusted as we go from  $N$  to  $K$  in order to keep  $v$  constant),

$$F_N(v) = (\Psi_N^0, \hat{h}\Psi_N^0) \text{ and } F_K(v) = (\Psi_K^0, \hat{h}\Psi_K^0),$$

and from Eqs. (1.5) and (1.6) we have

$$E_K^i = -\frac{(K-1)\hbar^2}{ma^2} (\Psi_K^i, \hat{h}\Psi_K^i) \leq E_K^{i+1}. \tag{2.5}$$

The right-hand side of Eq. (2.4) is therefore bounded above by the largest term  $(\Psi_K^0, \hat{h}\Psi_K^0)$  weighted by  $\sum_i |C_i|^2 = 1$  and consequently we obtain the required inequality (2.1).

Although we shall be using this result principally with  $K = 2$ , the geometrical property that the energy trajectories do not intersect often increases the value of any information we may obtain concerning the energy of the  $N$ -boson problem. If, for example, for a given  $f$ ,  $N$ ,  $V_0$ , and  $a$  we have calculated a variational upper bound  $E_U$  to  $E_N(a, V_0)$ , then we obtain a single point, say  $P_1 = (v_1, \epsilon_1)$  in the  $(v, \epsilon)$  plane, where by Eq. (1.5)  $v_1 = NmV_0\alpha/2\hbar^2$  and  $\epsilon_1 = -mE_U\alpha^2/(N-1)\hbar^2$ . Since  $P_1$  lies below the trajectories  $F_K$  for  $K \leq N$  (see Fig. 1 for an illustration of the geometry), we may conclude for each  $K \leq N$  and for all  $\lambda > 0$

$$\left(\frac{N-1}{K-1}\right) E_K(\lambda a, NV_0/K\lambda^2) \leq \frac{1}{\lambda^2} E_U. \tag{2.6}$$

Results similar to Eq. (2.6) have been discussed by Calogero *et al.*<sup>15</sup> and Balbutsev *et al.*<sup>16</sup>

We now turn to the "upper-bound" trajectory  $F_g$ . The use of Gaussian trial functions leads to an  $N$ -independent trajectory bound because of the unique factoring property<sup>9,10</sup> that a boson function  $\Phi$  of Jacobi coordinates factors in the form

$$\Phi(\vec{\rho}_2, \vec{\rho}_3, \dots, \vec{\rho}_N) = \phi(\vec{\rho}_2) G(\vec{\rho}_3, \vec{\rho}_4, \dots, \vec{\rho}_N)$$

if, and only if,  $\Phi$  is Gaussian. Since  $\langle H \rangle = \langle \mathcal{H} \rangle$ ,

we need only integrate over  $\vec{\rho}_2$ ; and for central potentials the problem reduces further to an integration over a single real variable. For a given  $v$  the formulas for  $F_g$  become

$$F_g(v) = \min_{\sigma} \epsilon(\sigma, v), \quad (2.7)$$

where

$$\begin{aligned} \epsilon(\sigma, v) &= (\phi, \hat{h}\phi) \|\phi\|^{-2} \\ &= -\frac{3}{4\sigma^2} + \left(\frac{2}{\pi}\right)^{1/2} v \int_0^{\infty} t^2 e^{-t^2/2} f(\sigma t) dt, \end{aligned} \quad (2.8)$$

and

$$\phi(x) = \exp[-(x/2\sigma)^2].$$

For a given value of  $v$ ,  $\epsilon(\sigma, v)$  is an integral transform of  $f(x)$ ; for a given value, say,  $\sigma_1$  of  $\sigma$ ,  $\epsilon(\sigma_1, v)$  is a linear function of  $v$  which is tangential to the optimal curve  $F_g$ . The linear trajectory bound

$$\epsilon(\sigma_1, v) \leq F_g(v) \leq F_N(v), \quad N \geq 2 \quad (2.9)$$

is extremely useful in actual calculations and we have earlier called this the tangent method (Ref. 17, Sec. 3.2).

Some other potential shapes for which the trajectory bounds  $F_2$  and  $F_g$  have been found are as follows: square,<sup>2</sup> exponential,<sup>2,12</sup> Hulthén,<sup>2</sup> Gauss,<sup>2</sup>  $\delta$  function,<sup>8</sup> Yamaguchi,<sup>11,17</sup> and logarithmic<sup>18</sup>; power-law potentials are discussed in Sec. III of this paper.

For linear transformations  $\alpha + \beta f$  of the potential shape  $f$ , the trajectory bounds  $F_2$  and  $F_g$  obey the general rule

$$F^{(\alpha+\beta f)}(v) = \alpha v + F^{(f)}(\beta v), \quad \beta > 0. \quad (2.10)$$

### III. POWER-LAW POTENTIALS

For power-law potentials we write

$$f(x) = -\text{sgn}(p)x^p, \quad p \neq 0. \quad (3.1)$$

It follows from Sec. II by use of the simple scale change of variables  $x' = v^{-1/(p+2)}x$  that the trajectory bounds  $F_2$  and  $F_g$  for these power-law potentials are given by

$$F_2^{(p)}(v) = F_2^{(p)}(1)v^{2/(p+2)}, \quad p \neq 0, \quad p > -2 \quad (3.2)$$

and

$$F_g^{(p)}(v) = F_g^{(p)}(1)v^{2/(p+2)}, \quad p \neq 0, \quad p > -2 \quad (3.3)$$

where  $F_2^{(p)}(1)$  is the largest eigenvalue of  $\hat{h} = \Delta - \text{sgn}(p)x^p$  and  $F_g^{(p)}(1)$  is the maximum expectation of  $\hat{h}$  with respect to normalized Gaussian functions of  $\vec{x}$ . For  $p < -2$  the wave functions must vanish sufficiently fast as  $x \rightarrow 0$  and this makes the Gaussian functions which we use for  $F_g$  unsuitable. The cases  $p=2$  (harmonic oscillator),  $p=1$  (linear potential<sup>19</sup>), and  $p=-1$  (hydrogen atom) are standard elementary problems for which we present  $F_2$  and  $F_g$  [along with the corresponding  $\gamma_2$  and  $\gamma_g$  for Eq. (1.12)] in Table I. The number given for  $F_2^{(1)}(1)$  is an approximation for the first zero of the Airy function.<sup>19</sup> From Eq. (2.7) we obtain the values of  $F_g^{(p)}(1)$  as follows:

$$F_g^{(p)}(1) = -3(p+2)/4p\sigma_1^2, \quad (3.4)$$

where

$$\sigma_1 = \left[ |p| 2^{(p+4)/2} \Gamma\left(\frac{3+p}{2}\right) / 3\pi^{1/2} \right]^{-1/(p+2)}, \quad p > -2, \quad p \neq 0.$$

The value

$$\sigma = \sigma_1 v^{-1/(p+2)} \quad (3.5)$$

determines via Eq. (2.8) the best  $N$ -body Gaussian trial wave function (with respect to energy) for the corresponding power-law potential. For the class of potentials (3.1) with  $p > -2$  and  $p \neq 0$ , the exact energy of the  $N$ -boson problem is therefore given by the expression

$$\epsilon = \frac{1}{2} [F_2^{(p)}(1) + F_g^{(p)}(1)] v^{2/(p+2)} \pm \delta\%, \quad (3.6)$$

where

$$\delta = 100 \left| \frac{F_2^{(p)}(1) - F_g^{(p)}(1)}{[F_2^{(p)}(1) + F_g^{(p)}(1)]^{-1}} \right|. \quad (3.7)$$

Thus, for example, if  $p=2$ ,  $F_2(v) = \epsilon$  is exact and  $\delta=0$ ; for  $p=1$ ,  $\delta < 0.15\%$ ; and for  $p=-1$ ,  $\delta < 8.1\%$ . These results which are valid for all  $N \geq 2$  provide useful tests for alternative approaches to the solution of the  $N$ -body problem. Our general formula Eq. (1.12) (yet to be proved) also yields Eqs. (3.2) and (3.3) as the special case in

TABLE I.  $F$  and  $\gamma$  numbers for problems in three dimensions.

Enveloping family	$p$	$F_2^{(p)}(1)$	$F_g^{(p)}(1)$	$\gamma_2(p)$	$\gamma_g(p)$
Hyperbolic	-1	$\frac{1}{4}$	$2/3\pi$	2	$3\pi/4$
Linear	1	-2.338 107	$-3(3/2\pi)^{1/3}$	3.787 210	$12/\pi$
Parabolic	2	-3	-3	$\frac{9}{2}$	$\frac{9}{2}$

which  $f$  is a power-law potential. The addition of a constant term to  $f$  leading to potentials which shapes like  $(1-x)$  for example can be treated by using the general rule Eq. (2.10). Thus we have for  $f(x) = (1-x)$

$$\epsilon = v - (2.341\,442\,5)v^{2/3} + \text{error}, \quad (3.8)$$

where

$$|\text{error}| < (0.004)v^{2/3}, \quad \text{all } v > 0$$

and

$$|\text{error}| < (0.005)|\epsilon|, \quad 0 < v < 4.7.$$

Equation (3.8) therefore represents an extremely accurate solution to the  $N$ -boson problem in the case of linear pair potentials.

#### IV. THE METHOD OF POTENTIAL ENVELOPES

Consider a monotone decreasing smooth potential shape  $f$ . Such a function is equal to the envelope of its tangents and for  $f'(s) < 0$ , the corresponding tangent line  $f_s(x)$  at the point  $x=s$  may be regarded as an attractive linear potential. Since we have been able to treat the  $N$ -boson problem with linear pair potentials very effectively, it is natural to hope that the representation of  $f$  as the envelope of a family of linear potentials may help us to solve the  $N$ -boson problem in which the pair potential has the shape  $f$ . Suppose for  $s \in S$  (where  $S$  is an interval) we have  $f'(s) < 0$  and  $f_s(x) \geq f(x)$ , for all  $x > 0$ , then every such linear potential  $f_s$  is a stronger potential (i.e., gives more binding) than  $f$  and we have

$$\epsilon \leq F_2^{(f_s)}(v), \quad s \in S.$$

An even better bound on  $\epsilon$  is provided by using the envelope of the family of trajectories  $\{F_2^{(f_s)}\}$  which we write as

$$F_L = \text{envelope}_{s \in S} \{F_2^{(f_s)}\}.$$

Thus, we have  $\epsilon \leq F_L(v)$ . By a similar argument in which we assume  $f_s(x) \leq f(x)$  for all  $x > 0$ , we obtain the corresponding bound  $\epsilon \geq F_U(v)$ . The *method of potential envelopes* is a generalization of this idea.

Suppose  $f$  is the potential shape we wish to study and suppose  $\phi$  is a potential shape for which we have already found the trajectory bounds  $F_2^{(\phi)}$  and  $F_g^{(\phi)}$ . We shall assume that  $f$  and  $\phi$  have continuous second derivatives and are compatible in the sense that  $f'(x)/\phi'(x) > 0$  for all  $x > 0$ . The smoothness assumption of  $f$  can be weakened if we confine our analysis to smooth patches of  $f$  lying between corners. We define the function  $g$  and the variable  $t$  as follows:

$$f(s) = g(\phi(s)), \quad t = \phi(s), \quad s > 0 \quad (4.1)$$

and we note that  $g'(t) = f'(s)/\phi'(s) > 0$  by our hypothesis. We now assume that for  $s \in S$  (or equivalently  $t \in T$ )

$$\begin{aligned} f(x) &= g(\phi(x)) \\ &\leq \phi_t(x) \equiv [g(t) - tg'(t)] + \phi(x)g'(t), \quad \text{all } x > 0. \end{aligned} \quad (4.2)$$

For this inequality to be valid for  $s \in S$  it is *necessary* that  $g''(\phi(s)) < 0$  for  $s \in S$  and this condition is also *sufficient* if  $S$  happens to be the half-line  $s > 0$ . The expression for  $g''(t)$  may be written as

$$\{\phi'(s)\}^2 g''(t) = f''(s) - f'(s)\phi''(s)/\phi'(s). \quad (4.3)$$

Since  $g'(t) > 0$ , the right-hand side of Eq. (4.2) represents a stronger potential than  $f$  and we have

$$\epsilon \leq F_L(v), \quad (4.4)$$

where

$$F_L = \text{envelope}_{t \in T} \{F_2^{(\phi_t)}\}, \quad (4.5)$$

and by Eq. (2.10)

$$F_2^{(\phi_t)}(v) = [g(t) - tg'(t)]v + F_2^{(\phi)}(g'(t)v). \quad (4.6)$$

In order to find  $F_L$  we must therefore solve Eq. (4.6) simultaneously with its partial derivative with respect to  $t$ , that is to say, with

$$0 = -tg''(t)v + F_2^{(\phi)'}(g'(t)v)g''(t)v,$$

i.e.,

$$t = F_2^{(\phi)'}(g'(t)v). \quad (4.7)$$

In order to find  $F_U$  where

$$\epsilon \geq F_U(v), \quad (4.8)$$

we repeat the above steps but reverse the inequality in Eq. (4.2) [implying now that  $g''(\phi(s)) > 0$ ,  $s \in S$ ], and replace each  $F_2^{(\phi)}$  by  $F_g^{(\phi)}$ .

We now apply this general analysis to the power-law potentials which we have studied in Sec. III:

$$\phi(x) = -\text{sgn}(p)x^p, \quad p \geq -1, \quad p \neq 0 \quad (4.9)$$

and

$$F^{(\phi)}(v) = F^{(\phi)}(1)v^{2/(\phi+2)}, \quad (4.10)$$

where the subscripts 2 and  $g$  are used on  $F$  as required. For this collection of curves the factor  $g'(t)$  becomes

$$tg'(t) = tf'(s)/\phi'(s) = p^{-1}sf'(s). \quad (4.11)$$

Consequently, Eqs. (4.5) and (4.6) for either  $F_L$  or  $F_U$  may be written in the following simple generic form.

*Formula for the trajectory bounds*

$$F(v) = \frac{1}{2}v[2f(s) + sf'(s)], \quad (4.12)$$

$$v = -\gamma(p)[s^3f'(s)]^{-1}, \quad s \in S$$

where for  $F_L$  and  $F_U$  we use, respectively, the positive constants  $\gamma_2(p)$  and  $\gamma_g(p)$  given for  $p \neq 0$ ,  $p \geq -1$  by

$$\gamma_2(p) = |p| \left| \frac{2F_2^{(p)}(1)}{(p+2)} \right|^{(2+p)/p}, \quad (4.13)$$

$$\gamma_g(p) = |p| \left| \frac{2F_g^{(p)}(1)}{(p+2)} \right|^{(2+p)/p}, \quad (4.14)$$

and

$$\gamma_g(2\nu) = \frac{3}{2}[3 \times 5 \times \cdots \times (2\nu+1)]^{1/\nu}, \quad \nu = 1, 2, 3, \dots$$

We observe that if we make the formal substitution  $f(s) = \phi(s)$  in Eq. (4.12), then the constants  $\gamma_2$  and  $\gamma_g$  are precisely the factors needed so that Eq. (4.12) yields Eq. (4.10) for the corresponding power-law potential. Some values for  $\gamma_2(p)$  and  $\gamma_g(p)$  are given in Table I.

For power-law envelopes the condition  $f'(s)/\phi'(s) > 0$  implies  $f'(s) < 0$ , i. e.,  $f$  must be monotone decreasing for such representations of  $f$ . The necessary conditions  $g''(t) < 0$  for  $F_L$  and  $g''(t) > 0$  for  $F_U$  become via Eqs. (4.3) and (4.9), respectively,  $D_p(s) \equiv [sf''(s) - (p-1)f'(s)] < 0$  and  $D_p(s) > 0$ , for  $s \in S$ . We may therefore summarize (for a given fixed value of  $p$ ) the conditions for the application of the formula (4.12) for the trajectory bounds as follows.

*Sufficient conditions for the trajectory-bound formula*

$$f'(x) < 0, \quad x > 0 \quad (4.15a)$$

$$F_L: D_p(s) \equiv [sf''(s) - (p-1)f'(s)] < 0, \quad s \in S \quad (4.15b_1)$$

$$F_U: D_p(s) \equiv [sf''(s) - (p-1)f'(s)] > 0, \quad s \in S \quad (4.15b_2)$$

$$F_L: f(x) < f_s(x) \equiv [f(s) - p^{-1}sf'(s)] + p^{-1}sf'(s)(x/s)^p \text{ each } s \in S, \text{ all } x > 0 \quad (4.15c_1)$$

$$F_U: f(x) > f_s(x) \equiv [f(s) - p^{-1}sf'(s)] + p^{-1}sf'(s)(x/s)^p \text{ each } s \in S, \text{ all } x > 0. \quad (4.15c_2)$$

$$\text{If } S = \{s \mid s > 0\}, \text{ then } b_1 \Rightarrow c_1 \text{ and } b_2 \Rightarrow c_2. \quad (4.16)$$

Equation (4.16) is proved, as in the general case, by first writing the difference  $\Delta(\phi) = f_s(x) - f(x)$ , for a given  $s$ , as a function of  $\phi(x)$  and observing that  $\Delta(t) = \Delta'(t) = 0$ ; condition (4.15b<sub>1</sub>) for all  $s > 0$  then implies via Eq. (4.3) that  $\Delta''(\phi(x)) > 0$ , that is to say,  $\Delta(\phi) \geq 0$ ; similarly (4.15b<sub>2</sub>)  $\Rightarrow$  (4.15c<sub>2</sub>).

We shall see in Sec. V that, for suitable choices of  $p$ , conditions (4.15b<sub>1</sub>) or (4.15b<sub>2</sub>) are often met

for all  $s > 0$  for large classes of potentials and consequently the corresponding trajectory bounds can immediately be found with ease by use of the generic formula Eq. (4.12). In cases where (4.15b<sub>1</sub>) or (4.15b<sub>2</sub>) are only satisfied for  $s$  in a finite interval  $S$ , the global conditions (4.15c<sub>1</sub>) or (4.15c<sub>2</sub>) must be examined independently.

We are now in a position to make some interesting general remarks about the shapes of the trajectory bounds  $F_L$  and  $F_U$  for a given potential shape  $f$ . Suppose that the choice  $p = p_1$  leads to  $F_L$  and  $p = p_2$  leads to  $F_U$ , then  $F_U$  is a magnification of  $F_L$  for if  $(v, \epsilon)$  is a point of  $F_L$ , then  $(\mu v, \mu \epsilon)$  is a point of  $F_U$  where  $\mu = \gamma_g(p_2)/\gamma_2(p_1) \geq 1$ . We know that  $\mu = 1$  only for the harmonic-oscillator potential with  $p_1 = p_2 = 2$ ; in general  $p_1 < p_2$ . If we define  $r(s)$  by

$$r(s) = 2f(s) + sf'(s), \quad s \in S \quad (4.17)$$

then we obtain from Eqs. (4.12) and (4.15b<sub>1</sub>) the following differential relations which are valid for both  $F_L$  and  $F_U$  when the appropriate  $\gamma > 0$  is used:

$$\frac{dv}{ds} = \gamma^{-1}(sv)^2 r'(s),$$

$$\frac{d\epsilon}{dv} = f(s), \quad (4.18)$$

$$\frac{d^2\epsilon}{dv^2} = \gamma(sv)^{-2} f'(s)/r'(s),$$

$$r'(s) = D_p(s) + (2+p)f'(s).$$

Since  $p > -2$  and  $f'(s) < 0$ , and since for  $F_L$  we have  $D_{p_1}(s) < 0$ , we conclude that  $r'(s) < 0$ ; for  $F_U$  we have  $D_{p_2}(s) > 0$ , but  $r'(s)$  is unchanged and therefore still negative. Consequently, we have the following general properties for both  $F_L$  and  $F_U$ :

$$\frac{dv}{ds} < 0, \quad \frac{d\epsilon}{dv} = F'(v) = f(s), \quad \frac{d^2\epsilon}{dv^2} = F''(v) > 0. \quad (4.19)$$

Thus, the trajectory bounds are concave up and therefore lie above their tangents. This is the property which allows us to use the *tangent method*<sup>17</sup> for approximating  $F_g$ : each Gaussian trial function with a fixed scale parameter  $\sigma$  provides a tangent line [Eq. (2.8)] to  $F_g$  which line is itself a trajectory bound; all the exact trajectories  $F_N$  lie above every member of this family of straight lines.

## V. SOME ILLUSTRATIONS

We choose classes of potential shapes so that within a class we have  $D_{p_1}(s) < 0$  and  $D_{p_2}(s) > 0$  for all  $s > 0$  for suitable fixed  $p_1$  and  $p_2$ . Con-

sequently, the trajectory bounds  $F_L$  and  $F_U$  are given for the whole  $(p_1, p_2)$  class by the general formula Eq. (4.12) with, respectively,  $\gamma = \gamma_2(p_1)$  and  $\gamma = \gamma_g(p_2)$  as given in Table I, or by Eqs. (4.13) and (4.14). The class magnification factor  $\mu$  is given by  $\mu = \gamma_g(p_2)/\gamma_2(p_1)$ . Two potential parameters,  $V_0$  and  $a$ , are always allowed for in our formulation because  $V(r_{ij}) = -V_0 f(r_{ij}/a)$ ; other parameters are introduced in the definition of each class of potential shapes. The classes, which are merely concrete illustrations, can be considerably enlarged.

A. Hyperbolic-linear:  $(p_1, p_2) = (-1, 1)$

Suppose  $f(x)$  is given by

$$f(x) = \frac{\alpha_1}{x} + \frac{\alpha_2}{x + \alpha_3} - \alpha_4 \ln x - \alpha_5 \operatorname{sgn}(q)x^q, \quad (5.1)$$

where  $\alpha_i \geq 0$  and  $|q| \leq 1$ . For this class of problems we may use the trajectory-bound formula Eq. (4.12) with  $\gamma = \gamma_2(-1) = 2$  and  $\gamma = \gamma_g(1) = 12/\pi$ , respectively, for  $F_L$  and  $F_U$ ; the magnification factor is  $\mu = 6/\pi$ . Thus, we can immediately determine how the energy of the  $N$ -boson system depends on  $N$  and all the potential parameters. The shifted Coulomb potential<sup>20</sup>  $f(x) = (1+x)^{-1}$  and the central term of a possible quark-quark potential<sup>14, 18</sup>  $f(x) = x^{-1} - \ln x - x$  are illustrated in Figs. 2 and 3; in Fig. 3 we have added the best Gaussian  $U$  trajectory determined by Eq. (2.7) and labeled by  $G$ ;  $F_L$  may also be

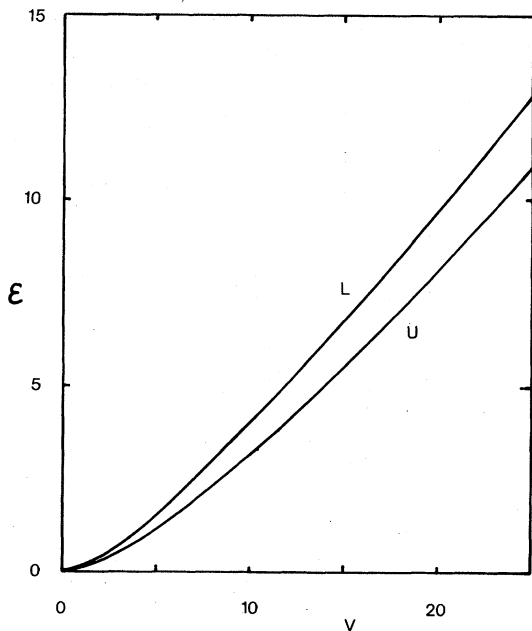


FIG. 2. Trajectory bounds for the shifted Coulomb potential with shape  $f(x) = (x+1)^{-1}$  in three dimensions:  $F_U(v) \leq \epsilon \leq F_L(v)$ .

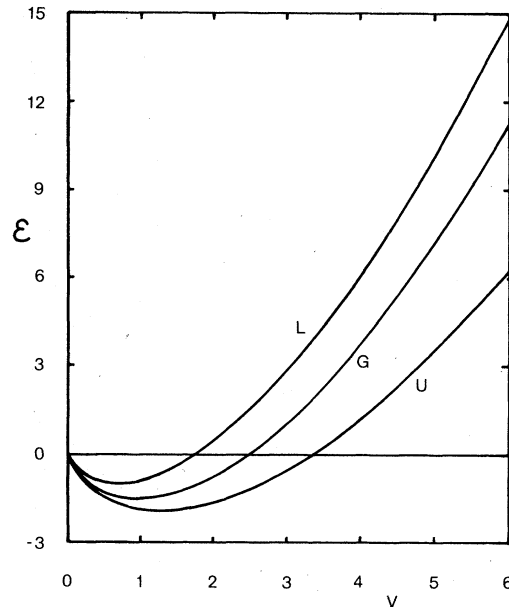


FIG. 3. Trajectory bounds for the quark-quark potential with shape  $f(x) = x^{-1} - \ln x - x$  in three dimensions: the curve labeled  $G$  is the best  $U$  trajectory which can be obtained by the use of a Gaussian trial function;  $F_U(v) < F_g(v) \leq \epsilon \leq F_L(v)$ .

improved by solving the two-body problem numerically. However, the main point of the envelope method is to provide a simple answer to the question: How does  $E_N$  depend on  $N$  and the potential parameters? For example, for the case  $f(x) = (1+x)^{-1}$  we have  $V(r_{ij}) = -(V_0 a)(r_{ij} + a)^{-1}$ , and for each choice of  $N \geq 2$ ,  $a > 0$ , and  $V_0 > 0$  we obtain a value for  $v = Nma^2/2\hbar^2$ ; the exact quantity  $-mE_N a^2/(N-1)\hbar^2$  then lies between  $F_L$  and its magnification by  $\mu = 6/\pi$ , where in this example  $F_L$  has the simple parametric form  $\{2(1+s)^2 s^{-3}, (2+s)s^{-3}\}$  for  $s > 0$ . Most of our illustrations have the same flavor as this example and they represent the nearest we have yet come to providing a recipe solution to the  $N$ -boson problem.

The exponential potential shape  $f(x) = e^{-x}$  lies above its tangents so that Eq. (4.12) yields  $F_U$  for  $p_2 = 1$ . However, if we write  $e^{-x}$  as the envelope of a family  $\{f_s\}$  of hyperbolas ( $p_1 = -1$ ), the hyperbola tangential at  $x = s$ , necessarily crosses  $f$  if  $s > 1$ ; consequently, we only obtain a partial  $F_L$  trajectory via Eq. (4.12) in this case, namely, for the values  $v \geq 2e$ , corresponding to  $s \leq 1$ . More explicitly, we have for the potential shape  $f(x) = e^{-x}$ :

$$F_L: \begin{cases} \epsilon = \frac{1}{2} v e^{-s} (2-s), \\ v = 2e^s / s^3, \quad 0 < s \leq 1 \end{cases}$$

and

$$F_U: \begin{cases} \epsilon = \frac{1}{2} v e^{-s} (2 - s), \\ v = 12 e^s / \pi s^3, \quad s > 0. \end{cases}$$

We have earlier obtained<sup>2</sup> very accurate results for this potential but the present partial and rather less accurate results are certainly delightfully easy to find.

**B. Hyperbolic-parabolic:  $(p_1, p_2) = (-1, 2)$**

This class of potentials includes all those of class (A) plus terms, for example, of the form

$$f(x) = -x^2 + \frac{\lambda x^2}{(1 + g x^2)}, \quad (5.2)$$

where  $g \geq 0$  and  $0 \leq \lambda \leq 9$ . The upper limit on  $\lambda$  is sufficient to guarantee  $D_{-1}(s) < 0$ , and  $D_2(s) > 0$  for all  $s > 0$ . For this class of shapes we have for  $F_L$  and  $F_U$ , respectively,  $\gamma = \gamma_2(-1) = 2$  and  $\gamma = \gamma_g(2) = \frac{9}{2}$ , so that  $\mu = \frac{9}{4}$ .

We can also discuss the Gauss-well  $f(x) = e^{-x^2}$  with these  $\gamma$  numbers, but, as with the exponential potential in class (A), the  $F_L$  curve is only obtained in part, namely, for  $v \geq 4e^{1/2}$ , corresponding to  $s \leq 1/\sqrt{2}$ .

**C. Linear-parabolic:  $(p_1, p_2) = (1, 2)$**

We now consider perturbed harmonic oscillators with the forms

$$f(x) = -(x^2 + \alpha e^{-x^2}), \quad 0 \leq \alpha \leq 1 \quad (5.3)$$

and

$$f(x) = -\left(x^2 + \frac{\lambda x^2}{1 + g x^2}\right), \quad 0 \leq \lambda \leq 3, \quad g \geq 0. \quad (5.4)$$

The parameters  $\alpha$  and  $\lambda$  have been restricted so that  $D_1(s) < 0$  and  $D_2(s) > 0$  for all  $s > 0$  (the parameters  $V_0$  and  $a$  are still free). Consequently, we may find trajectory bounds via Eq. (4.12) in which  $\gamma = \gamma_2(1) = 3.78721$  for  $F_L$  and  $\gamma = \gamma_g(2) = \frac{9}{2}$  for  $F_U$ , so that  $\mu = 1.1882$ . The case  $\lambda = g = 1$  of the potential shape Eq. (5.4) is illustrated in Fig. 4. Since for the special case  $N=2$  the lowest eigenvalue of  $\hat{h}$  is equal to the energy of the first excited state of the corresponding problem in *one* spatial dimension, we also display in Fig. 4 the results for this latter problem computed by Mitra<sup>21</sup> (using a variational method) and Kaushal<sup>22</sup> (using perturbation theory). In order to represent the results of these authors in our notation we have had to derive the following scaling law:

$$\epsilon = F(v, \lambda, g) = v^{1/2} F(1, \lambda, g/v^{1/2}). \quad (5.5)$$

Our results have been obtained by an application of the very general recipe Eq. (4.12) for the energy of the  $N$ -boson problem for *all*  $N$  and naturally we should not expect to compete in terms of accuracy with the results of special studies of the

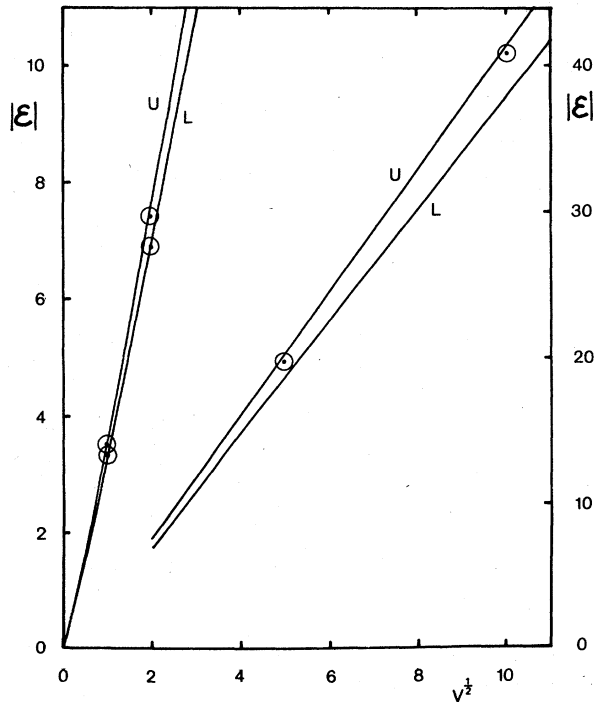


FIG. 4. Trajectory bounds for the perturbed harmonic oscillator with shape  $f(x) = -[x^2 + x^2(1 + x^2)^{-1}]$  in three dimensions. The points  $\odot$  are the energies of the first excited state of the *two*-body problem in one dimension obtained by Mitra (Ref. 21) and Kaushal (Ref. 22); for  $v^{1/2} = 1$  and 2, these values differ significantly and the upper points are those of Mitra (see the text for more accurate data).

*two*-body problem for a given interaction. However, for perturbation methods such as in Ref. 22, our *strict* upper and lower bounds may still be of interest, as a check, even for  $N=2$ . With  $\lambda = g = 1$  and  $v = 1$  and  $v = 4$ , for example, the sequences of estimates ( $|F_L(v)|$ , Kaushal,<sup>22</sup> Mitra,<sup>21</sup>  $|F_U(v)|$ ) for  $|\epsilon|$  are, respectively, (3.220, 3.305, 3.507, 3.589) and (7.053, 6.918, 7.428, 7.637).

**D. Harmonic-power ( $2\nu$ ):  $(p_1, p_2) = (2, 2\nu)$**

As a final illustration of problems in three dimensions we consider perturbed harmonic oscillators of the form

$$f(x) = -(x^2 + \lambda x^{2\nu}), \quad \lambda \geq 0, \quad \nu = 1, 2, 3, \dots \quad (5.6)$$

For potential shapes of this kind we can find energy trajectories via Eq. (4.12) with  $\gamma = \gamma_2(2) = \frac{9}{2}$  for  $F_L$  and [see Eq. (4.14)]  $\gamma = \gamma_g(2\nu) = \frac{3}{2} [3 \times 5 \times \dots \times (2\nu + 1)]^{1/\nu}$  for  $F_U$ . Since our parameters  $a$  and  $V_0$  are still free,  $\lambda$  is actually redundant and we may therefore set  $\lambda = 1$ . The case  $f(x)$



$=(x^2+x^4)$  has the magnification factor  $\mu=1.291$ . Examples such as  $f(x)=-(x^2+\lambda x^4+\alpha x^6)$  are treated by taking  $\gamma_2(2)=\frac{9}{2}$  for  $F_L$  and  $\gamma_g(6)=\frac{3}{2}(105)^{1/3}$  for  $F_U$ : the magnification factor in this case becomes  $\mu=1.570$ .

## VI. PROBLEMS IN ONE DIMENSION

For symmetric potentials with shape  $f$  in one dimension the operator corresponding to  $\hat{h}$  in Eq. (1.5) becomes

$$\hat{h}=\frac{d^2}{dx^2}+vf(|x|). \quad (6.1)$$

All our general arguments go through in the same fashion for problems in one dimension. However, there are some differences of detail which we now discuss. The power laws  $f(|x|)=|x|^p$  for  $p < 0$  require a special vanishing condition on the wave function at  $x=0$  and consequently we cannot use families of such functions to model a nonsingular potential because the problems have different Hilbert spaces: thus, for nonsingular potentials, hyperbolic envelopes ( $p=-1$ ) are *not* generally useful in one dimension. For the familiar Coulomb case in three dimensions it is the product  $r\Psi(r)$  which must vanish at the origin: the radial wave function  $\Psi(r)$  itself is, of course, like  $e^{-kr}$ .

The Schrödinger equation for the linear potential in one dimension may be written

$$\Psi''(x)-(\epsilon+vx)|\Psi(x)=0. \quad (6.2)$$

If we make the change of variables (for  $x \geq 0$ )

$$\xi=v^{-2/3}(\epsilon+vx) \text{ and } \Psi(x)=\phi(\xi), \quad (6.3)$$

then Eq. (6.2) becomes Airy's equation

$$\phi''(\xi)-\xi\phi(\xi)=0. \quad (6.4)$$

The continuity of  $\Psi'(x)$  at  $x=0$  implies

$$\phi'(e v^{-2/3})=\text{Ai}'(e v^{-2/3})=0 \quad (6.5)$$

and we see that the product  $e v^{-2/3}$  is equal to the first zero of the derivative of Airy's function,<sup>23</sup> that is to say, we have for the exact ground-state solution of the two-body problem

$$\epsilon=F_2^{(1)}(v)=-1.0879297v^{2/3}. \quad (6.6)$$

If we now use a Gaussian trial wave function  $\phi(x)$

$=\exp\{-x^2/2\sigma^2\}$  to estimate  $\epsilon$  we find

$$\epsilon \geq F_g^{(1)}(v)=-\frac{3}{2}\pi^{-1/3}v^{2/3}. \quad (6.7)$$

If  $v$  and  $\epsilon$  are again taken to be as in Eq. (1.5), we have  $F_g^{(1)}(v) \leq \epsilon \leq F_2^{(1)}(v)$  for the  $N$ -boson problem with the linear pair potential in one dimension: this is, as we found in three dimensions, an accurate approximation since  $\frac{3}{2}\pi^{-1/3} \approx 1.024176$ .

For the harmonic oscillator  $f(x)=-x^2$  we have for the  $N$ -boson problem the *exact* solution

$$\epsilon=F_2^{(2)}(v)=F_g^{(2)}(v)=-v^{1/2}. \quad (6.8)$$

Some  $F$  numbers and  $\gamma$  numbers [obtained from the  $F$  numbers by Eqs. (4.13) and (4.14)] for problems in one dimension are shown in Table II. The generic formula Eq. (4.12) for the trajectory bounds and the sufficiency conditions Eq. (4.15) remain the same as in three dimensions. The  $\gamma_g$  numbers for  $p$  even are given in one dimension by the general formula

$$\gamma_g(2\nu)=\frac{1}{2}[1 \times 3 \times 5 \times \cdots \times (2\nu-1)]^{1/\nu}, \quad \nu=1,2,3,\dots \quad (6.9)$$

Since we have already illustrated the envelope method in Sec. V for problems in three dimensions we shall consider only one example here of a one-dimensional problem. Mitra<sup>21</sup> and Kaushal<sup>22</sup> have recently studied the *one*-particle problem (i.e., equivalently the reduced two-particle problem, or  $N=2$  in our formulation) with potential shape

$$f(x)=-\left(x^2+\frac{\lambda x^2}{1+gx^2}\right), \quad \lambda, g > 0.$$

As we saw in Sec. V, for us this is linear-parabolic problem provided  $\lambda \leq 3$  (for all  $g > 0$ ). Consequently, we obtain  $F_L$  by setting  $\gamma=\gamma_2(1)=0.313317$  and  $F_U$  by setting  $\gamma=\gamma_g(2)=0.5$  in Eq. (4.12), which provides a recipe for the ground-state energy of the  $N$ -boson problem as a function of  $\lambda$  and  $g$ . Some results for  $\lambda=g=1$  are shown in Fig. 5; in order to include the results of Refs. 21 and 22 we have again used the scaling law Eq. (5.5). The remarks made in Sec. V about ac-

TABLE II.  $F$  and  $\gamma$  numbers for problems in one dimension.

Enveloping family	$p$	$F_2^{(p)}(1)$	$F_g^{(p)}(1)$	$\gamma_2(p)$	$\gamma_g(p)$
Linear	1	-1.018 793	$-3\pi^{-1/3}/2$	0.313 317	$\pi^{-1}$
Parabolic	2	-1	-1	$\frac{1}{2}$	$\frac{1}{2}$

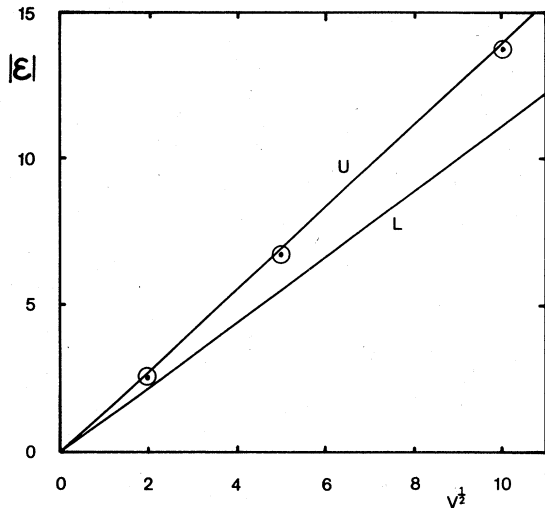


FIG. 5. Trajectory bounds for the perturbed harmonic oscillator with shape  $f(x) = -[x^2 + x^2(1+x^2)^{-1}]$  in one dimension. The points  $\odot$  are the energies of the *two*-body problem obtained by Mitra (Ref. 21) and Kaushal (Ref. 22).

curacy are also relevant here. In addition, we expect in general to obtain worse results in one dimension than in three dimensions because of the way the  $\gamma$  numbers vary. This can be seen, for example, if we compare Eq. (4.14) with Eq. (6.9): the  $(2, 2\nu)$  magnification factor  $\mu = \gamma_2(2\nu)/\gamma_2(2)$  is larger in one dimension than in three dimensions.

## VII. CONCLUSION

For an increasing potential  $V(r_{ij}) = -V_0 f(r_{ij}/a)$  which can be regarded as the envelope of a family of power-law potentials, we have discovered a simple universal formula Eq. (4.12) for the dependence of the energy of the  $N$ -boson problem on  $N$ ,  $V_0$ ,  $a$ , and the parameters of the potential shape  $f$ . Because the formula is simple to state and to use, we are hopeful that it may be employed as a tool with which to discuss the inverse problem of quantum mechanics: given  $E_N$ , find  $V$ .

Having established a general result like Eq. (4.12), we should expect that alternative proofs are available, and indeed this is the case. Since the  $L$  trajectories are obtained by an overall minimization of the energy expectation  $\langle \hat{h} \rangle$ , and the  $U$  trajectories are obtained by a minimization with respect to scale, both trajectories satisfy the virial theorem<sup>24</sup> and consequently we have

$$\langle \hat{h} \rangle = \langle \Delta_x + v f(x) \rangle = \frac{1}{2} v \langle 2f(x) + x f'(x) \rangle. \quad (7.1)$$

The passage from Eq. (7.1) to Eq. (4.12) can then be made, although by no means immediately, via

suitable integral inequalities. This alternative approach can also be used to strengthen the method in the following way: we select a class of potential shapes and then search for the best  $\gamma$  numbers,  $\gamma_L$  and  $\gamma_U$ , for this class. We have chosen to present our results in the geometrical and physical form in which they were discovered but further improvements may come in answer to purely mathematical questions concerning optimal  $\gamma$  numbers and integral inequalities.

The general envelope method, Eqs. (4.6) and (4.7), is *not*, of course, restricted to envelopes of families of power-law potentials. We have obtained similar results, for example, for families of square-well potentials and families of Hulthén potentials [i. e.,  $f(x) = e^{-x}(1 - e^{-x})^{-1}$ ]. However, once we leave the simple power-law collection of shapes, the peculiarities and intricacies of the corresponding sufficiency conditions would only be of interest in connection with a specific application.

For molecular forces such as those derived from the Lennard-Jones potential, the Gaussian trial function is not appropriate and instead one would have to use, for example, a more general Jastrow function<sup>25</sup> of the form  $\phi = \prod_{i < j} \Psi(r_{ij})$  with suitable  $\Psi$ . Jastrow functions are not only very useful,<sup>26</sup> but the two known soluble bound  $N$ -boson problems, the  $\delta$ -function potential in one dimension<sup>7</sup> and the harmonic oscillator, both happen to have exact ground states which are of this form; however, we have not been able to work with such trial functions for all  $N$  in general without making special approximations. A review of the literature concerning the quality of the lower bound for systems of particles interacting by molecular or nuclear forces may be found in a recent article by Hill.<sup>27</sup>

The aim of the present paper has been to exploit existing knowledge concerning the two-body eigenvalue problem for certain specific potentials in order to give information about the  $N$ -body problem in more general cases. We can summarize the principal ideas which we have used as follows.

(a) For the two-body system, each potential shape  $f$  leads to an energy trajectory  $F$  which describes how the energy depends on the coupling constant.

(b) In order to analyze the map  $\Lambda: f \rightarrow F$  we use, in place of the classical analytical tools of power series or Fourier series, a representation for  $f$  as the *envelope* of a family of well-understood potential shapes. This leads eventually to a recipe for upper and lower bounds to  $F$  given directly in terms of the potential shape  $f$  itself.

(c) The methods of Ref. 2 are applied to extend (a) and (b) to the  $N$ -body problem.

For the special case  $N=2$  the results we have given in this paper as illustrations may be strengthened since a Gaussian trial function is not required for  $F_V$ : specifically, we may replace  $\gamma_g(p)$  by  $\gamma_2(p)$  and, of course,  $\gamma_2(p) \leq \gamma_g(p)$  with equality only for  $p=2$ .

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