Comparison between the exact and Hartree solutions of a one-dimensional many-body problem

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The exact solution for the ground state of the quantum one-dimensional N-boson problem with attractive δ-function two-body potentials is compared with the (exact) self-consistent solution of the corresponding variational Hartree problem.

I. INTRODUCTION

The Hartree-Fock (for fermions) and the Hartree (for bosons) approximations play a fundamental role in the study of many-particle systems. The Raleigh-Ritz theorem implies that the solutions yielded by these approaches provide a rigorous upper bound to the exact ground-state energy of the system; but little is known about the accuracy of these approximate techniques,[1] their general acceptance resting largely on the apparent soundness of the physical picture that constitutes their basis. It is therefore of interest to compare the exact and approximate results in one case, in which both can be evaluated exactly. This test case is the one-dimensional problem of N bosons interacting via two-body δ-function potentials.[2] In this paper we report the results for the ground state in the attractive case; because this state is bound, no container is needed to confine the system, and this implies a considerable simplification. Indeed the N-body problem has been solved exactly only in this case. The Hartree problem can be solved exactly even in the presence of a container, but this problem (including the interesting questions of the dependence upon the boundary conditions and of the "thermodynamical" limit as the size of the container diverges proportionally to N) shall be discussed elsewhere.

II. EXACT SOLUTION

The Hamiltonian for the problem is[3]

$$H=-\sum_{i=1}^{N}\frac{\partial^2}{\partial x_i^2}-g\sum_{i>j=1}^{N}\delta(x_i-x_j),\quad g>0\ . \tag{1}$$

The exact ground state of this system is the (only) N-body bound state, and it is characterized by the (translation-invariant and symmetrical) N-particle wave function[2]

$$\psi_N=C_N\exp\left(-\frac{1}{4}g\sum_{i>j=1}^{N}|x_i-x_j|\right)\ . \tag{2}$$

In order that this wave function be normalized,

$$\int_{-\infty}^{+\infty}dx_1\cdots dx_N\,\delta(x_{\text{c.m.}})\,|\psi_N|^2=N\ , \tag{3}$$

the constant $|C_N|$ has the value (see Appendix A)

$$|C_N|=N!\,[(N-1)!\,(\tfrac{1}{2}g)^{N-1}]^{1/2}\ . \tag{4}$$

In Eq. (3), and always in the following,

$$x_{\text{c.m.}}\equiv\frac{1}{N}\sum_{i=1}^{N}x_i\ .$$

The density

$$\rho_N(x)=\int_{-\infty}^{+\infty}dx_1\cdots dx_N\,\delta(x_{\text{c.m.}})\delta(x_1-x)\,|\psi_N|^2 \tag{5}$$

corresponding to this N-particle state can also be evaluated exactly (see Appendix A):

$$\rho_N(x)=\frac{1}{2}g\sum_{n=1}^{N-1}(-)^{n+1}\frac{n(N!)^2e^{-gnN|x|/2}}{(N+n-1)!(N-n-1)!}\ . \tag{6}$$

The argument x of $\rho_N(x)$ represents of course the distance from the center-of-mass of the system. In the limit of large N, this formula yields (for $|x|>0$)

$$\rho_N(x)=\tfrac{1}{8}gN^2[\cosh(\tfrac{1}{4}gNx)]^{-2}\times\{1-N^{-1}[1-\tfrac{3}{2}\cosh^{-2}(\tfrac{1}{4}gNx)]+O[N^{-2},\,Ne^{-gN^2|x|/2}]\}\ . \tag{7}$$

As for the central density $\rho_N(0)$, it can be evaluated in closed form for all N (see Appendix A):

$$\rho_N(0)=\tfrac{1}{4}gN^2(N-1)/(2N-3)\ . \tag{8}$$

The ground-state energy of the system, corresponding to the wave function (2), is[2]

$$E_N = -\tfrac{1}{48} g^2 N(N^2-1) . \quad (9)$$

As a consequence of the purely attractive character of the forces, clearly in the limit of large N the system collapses to a (linear) volume of order $1/gN$ and the (binding) energy per particle is proportional to $(gN)^2$. It should be noted that the assumption that g be inversely proportional to N, $g=\gamma/N$ with γ constant, although implying a finite binding energy per particle in the limit of large N, does not prevent the collapse, since in the limit of large N the system would then reduce to a fixed size (of order $1/\gamma$), and its central density would diverge proportionally to N.[4]

III. SELF-CONSISTENT HARTREE SOLUTION

The Hartree (approximate) solution for the ground state of the problem obtains inserting in the Ritz variational principle,

$$E_N \leq E[\psi_t] \equiv (\psi_t | H - H_{\text{c.m.}} | \psi_t) , \quad (10)$$

the trial wave function[5]

$$\psi_t = N^{1/2} \prod_{i=1}^{N} \varphi(x_i) . \quad (11)$$

This trial wave function is not translation invariant, this being a well-known difficulty of the Hartree method. For this reason in (10) the center-of-mass Hamiltonian $H_{\text{c.m.}} = -N^{-1}(\partial^2/\partial x^2_{\text{c.m.}})$ has been subtracted from the N-body Hamiltonian (other prescriptions are discussed below).

The (normalized) single-particle wave function $\varphi(x)$ is determined so that the functional $E[\psi_t]$ attain its minimal value $E_N^{(H)}$, which represents the Hartree approximation (by excess) to the exact ground-state energy E_N. The process of minimization of the nonlinear functional of $\varphi(x)$ (which obtains by inserting (11) in $E[\psi_t]$) yields, by standard techniques, the Hartree eigenvalue equation[6]

$$-[(N-1)/N]\varphi''(x) - (N-1)g|\varphi(x)|^2\varphi(x) = \epsilon\varphi(x), \quad (12)$$

the value $E_N^{(H)}$ being then related to the smallest eigenvalue $\epsilon_{(N)}$ of this nonlinear equation by the relation

$$E_N^{(H)} = N\epsilon_{(N)} + \tfrac{1}{2}N(N-1)g\int_{-\infty}^{+\infty} dx\,|\varphi(x)|^4 . \quad (13)$$

The function $\varphi(x)$ appearing in this equation is of course the normalized "self-consistent" eigenfunction of (12) corresponding to the smallest eigenvalue $\epsilon_{(N)}$, and it is related to the (Hartree approximation for the) density $\rho_N^{(H)}(x)$ of the system by

$$\rho_N^{(H)}(x) = N|\varphi(x)|^2 . \quad (14)$$

As shown in Appendix B, the only[7] normalized solution of (12) is

$$\varphi(x) = (\tfrac{1}{8}gN)^{1/2}/\cosh(\tfrac{1}{4}gNx) , \quad (15)$$

and the corresponding eigenvalue is

$$\epsilon_{(N)} = -\tfrac{1}{16}g^2 N(N-1) . \quad (16)$$

Thus the Hartree method yields

$$E_N^{(H)} = -\tfrac{1}{48}(gN)^2(N-1) = E_N[N/(N+1)] \quad (17)$$

and

$$\rho_N^{(H)}(x) = \tfrac{1}{8}gN^2[\cosh(\tfrac{1}{4}gNx)]^{-2} , \quad (18)$$

implying

$$\rho_N^{(H)}(0) = \tfrac{1}{8}gN^2 = \rho_N(0)[(2N-3)/(2N-2)] . \quad (19)$$

IV. DISCUSSION

The comparison of the Hartree results with the exact ones is so explicit and simple as to require no comments. We merely emphasize that all Hartree results coincide with the exact ones in the limit of large N (even if g were assumed to depend on N, e.g., $g=\gamma/N$), while they may be quite off the mark for small N; this is consistent with the philosophy underlying the Hartree method, and may be largely traced to the non–translation-invariant character of the Hartree many-particle wave function.

Indeed, because the subtraction of the center-of-mass kinetic energy is an important, and contentious, issue in Hartree and Hartree-Fock computations of not-too-many-body systems,[8] it is of interest to mention the results (all of which can be easily computed in closed form) that would be obtained employing other (less accurate) prescriptions to subtract the contribution of the center-of-mass motion. The roughest procedure is to ignore altogether the problem, namely, omit to subtract $H_{\text{c.m.}}$ from H in Eq. (10). This results in the disappearance of the factor $(N-1)/N$ in the first term of the right-hand side of (12), yielding, in place of Eqs. (17)–(19), the results

$$E_N^{(H)} = -\tfrac{1}{48}g^2N(N-1)^2 = E_N[(N-1)/(N+1)] , \quad (20)$$

$$\rho_N^{(H)} = \tfrac{1}{8}gN(N-1)\{\cosh[\tfrac{1}{4}g(N-1)x]\}^{-2} , \quad (21)$$

and

$$\rho_N^{(H)}(0) = \tfrac{1}{8}gN(N-1) = \rho_N(0)[(2N-3)/(2N)] . \quad (22)$$

A less drastic procedure (often employed in actual computations) performs similarly the minimization procedure (ignoring the center-of-mass problem), but subsequently subtracts the expectation value of the center-of-mass Hamiltonian $H_{\text{c.m.}}$ (evaluated in the state described by the Hartree wave function that minimizes the expectation value of H). This procedure yields of course the same expressions (21) and (22) for the density, but a value for the energy intermediate between (20) and (17), namely,

$$E_N^{(H)} = -\tfrac{1}{48} g^2(N-1)^2(N+1) = E_N[(N-1)/N] . \tag{23}$$

Of course all these results coincide for large N. The difference $|E_N|/N(N+1)$ between (23) and (17) is a measure of the spuriosity[7] of the Hartree many-particle wave function (this difference would vanish were the dependence upon the center-of-mass coordinate factorable); it is smaller than the difference $|E_N|/(N+1)$ between (17) and (9) which accounts for *all* the inadequacies of the Hartree trial wave function and not only its lack of translational invariance.[9]

APPENDIX A

In Appendix A we prove Eqs. (4), (6), and (8).

We start with Eq. (5) of the density $\rho_N(x)$ which, using (2), can be rewritten as follows[10]:

$$\rho_N(x) = N|C_N|^2(2/g)^{N-2} I_N(\tfrac{1}{2}gx) , \tag{A1}$$

where

$$I_N(t) = \int_{-\infty}^{+\infty} dt_1 \cdots dt_N \delta\Big(\sum_{i=1}^N t_i\Big)\, \delta(t-t_1) \times \exp\Big(-\sum_{i>j=1}^N |t_i - t_j|\Big) . \tag{A2}$$

Clearly $I_N(t)$ is an even function of t; hereafter we assume, for simplicity, that t is nonnegative.

The symmetrical way the different coordinates enter in the definition of $I_N(t)$ (clearly any other coordinate could take the place of t_1 without changing the result) implies that we can write

$$I_N(t) = [N(N!)]^{-1} \sum_{n=1}^N I_{N,n}(t) , \tag{A3}$$

with

$$I_{N,n}(t) = \int_{-\infty}^{+\infty} dt_N \int_{-\infty}^{t_N} dt_{N-1} \cdots \int_{-\infty}^{t_2} dt_1 \delta\Big(\sum_{k=1}^N t_k\Big) \times \delta(t-t_n)\exp\Big(-\sum_{i>j=1}^N (t_i - t_j)\Big) . \tag{A4}$$

It is now convenient to introduce the Fourier transform of $I_{N,n}(t)$,

$$\hat{I}_{N,n}(\nu) = \int_{-\infty}^{+\infty} dt\, e^{-i\nu t} I_{N,n}(t) . \tag{A5}$$

Inserting in this formula the Fourier representation of the center-of-mass δ function,

$$\delta\Big(\sum_{k=1}^N t_k\Big) = (2\pi)^{-1} \int_{-\infty}^{+\infty} d\omega \exp\Big(i\omega \sum_{k=1}^N t_k\Big) , \tag{A6}$$

and introducing the constants α_k with the position

$$\sum_{i>j=1}^N (t_i - t_j) = \sum_{k=1}^N \alpha_k t_k , \tag{A7}$$

we then get

$$\hat{I}_{N,n}(\nu) = (2\pi)^{-1} \int_{-\infty}^{+\infty} d\omega \int_{-\infty}^{+\infty} dt_N \exp[(i\omega - \alpha_N)t_N] \int_{-\infty}^{t_N} dt_{N-1} \exp[(i\omega - \alpha_{N-1})t_{N-1}] \cdots \int_{-\infty}^{t_{n+1}} dt_n \exp[(i\omega - i\nu - \alpha_n)t_N] \cdots \int_{-\infty}^{t_2} dt_1 \exp[(i\omega - \alpha_1)t_1] \tag{A8}$$

$$= \int_{-\infty}^{+\infty} d\omega \Big(\prod_{j=1}^{N-1} \sum_{k=1}^{j} (i\omega - a_k^{(n)})\Big)^{-1} \delta\Big(\sum_{k=1}^N (\omega + i a_k^{(n)})\Big) \tag{A9}$$

$$= \Big(N \prod_{j=1}^{N-1} \sum_{k=1}^{i} (A^{(n)} - a_k^{(n)})\Big)^{-1} . \tag{A10}$$

In these expressions

$$a_k^{(n)} = \alpha_k + i\nu\delta_{k,n} , \tag{A11}$$

$$A^{(n)} = N^{-1} \sum_{k=1}^N a_k^{(n)} . \tag{A12}$$

The explicit expression of the coefficients α_k obtains easily from definition (A7). We find

$$\alpha_k = 2k - N - 1 , \tag{A13}$$

and from this it follows that $A^{(n)}$ is actually independent of the index n,

$$A^{(n)} = i\nu/N . \tag{A14}$$

Inserting these expressions in (A10) and performing the sums and products we get

$$\hat{I}_{N,n}(\nu)=\left(\frac{(-)^n i^{N+1}N^{N-2}}{(N-n)!\,(n-1)!}\right)\prod_{j=1}^{N-1}(\nu-\nu_j^{(n)})^{-1}\,. \tag{A15}$$

We now perform, using the residue theorem, the Fourier transform

$$I_{N,n}(t)=(2\pi)^{-1}\int_{-\infty}^{+\infty}d\nu\, e^{i\nu t}\hat{I}_{N,n}(\nu)\,, \tag{A16}$$

and we get

$$I_{N,n}(t)=(-)^{n+1}[(n-1)!\,(N-n)!\,]^{-1}\sum_{j=1}^{n-1}(-)^j(N+n-j-1)!\,e^{-N(N-j)t}/[(j-1)!\,(n-j-1)!\,(2N-j-1)!\,]\,. \tag{A17}$$

Inserting this expression in (A3) we obtain

$$I_N(t)=\sum_{m=1}^{N-1}I_m^{(N)}\,e^{-mNt}\,, \tag{A18}$$

with

$$I_m^{(N)}=(-)^{m+1}[N(N!)(N+m-1)!\,(N-m-1)!\,]^{-1}\sum_{k=0}^{m-1}(-)^k(N+m-1-k)!\,/[k!\,(m-1-k)!\,(N-1-k)!\,]\,. \tag{A19}$$

The sum in this expression can be performed using the Saalschütz formula,[11] getting

$$I_m^{(N)}=(-)^{n+1}m/[N!\,(N+m-1)!\,(N-m-1)!\,]\,. \tag{A20}$$

Thus, we finally obtain

$$\rho_N(x)=|C_N|^2(2/g)^{N-2}\sum_{n=1}^{N-1}(-)^{n+1}n\,e^{-gnN|x|/2}\,/[(N-1)!\,(N+n-1)!\,(N-n-1)!\,]\,. \tag{A21}$$

There remains to compute $|C_N|$, which is fixed by the normalization condition (3), or, equivalently, by the condition

$$\int_{-\infty}^{+\infty}dx\,\rho_N(x)=N\,. \tag{A22}$$

This becomes, upon integration of (A21),

$$|C_N|^{-2}=2(2/g)^{N-1}\sum_{n=1}^{N-1}(-)^{n+1}[N!\,(N+n-1)!\,(N-n-1)!\,]^{-1}\,. \tag{A23}$$

The sum on the right-hand side of (A23) can again be performed,[12] and there obtains expression (4) for $|C_N|$, that is thereby proved. Insertion of this expression for $|C_N|$ in (A21) then yields Eq. (6), that is thereby also proved.

The last equation to be proved is (8). This follows from (6), using again twice, after appropriate changes of indices, the same formula used to evaluate (A23).

APPENDIX B

In Appendix B we solve the Hartree eigenvalue equation (12).

We are interested in normalizable solutions, that must therefore vanish asymptotically. The structure of Eq. (12) immediately implies that the corresponding eigenvalue ϵ is negative and that asymptotically not only the solution φ, but also its derivatives, vanish (exponentially). From this remark there immediately follows that, apart from a constant phase factor, any normalizable solution φ of Eq. (12) is real. In fact inserting the polar representation

$$\varphi(x)=A(x)e^{i\chi(x)}\,, \tag{B1}$$

with $A(x)$ and $\chi(x)$ real, in Eq. (12), we get

$$-[(N-1)/N]\{A''(x)-[\chi'(x)]^2A(x)\}-(N-1)gA^3(x)=\epsilon A(x), \tag{B2}$$

and

$$\chi''(x)A(x)+2\chi'(x)A'(x)=0\,. \tag{B3}$$

The second equation can be immediately integrated, yielding

$$\chi'(x)=C[A(x)]^{-2}\,, \tag{B4}$$

C being an arbitrary (real) constant. Inserting this in (B2), we get

$$-[(N-1)/N][A''(x)-C^2A^{-3}(x)]-(N-1)gA^3(x)=\epsilon A(x)\,. \tag{B5}$$

Looking at this equation in the asymptotic region, we immediately conclude that the constant C must vanish, implying, through (B4), that $\chi(x)$ must be a constant. Q.E.D.

Neglecting hereafter a constant phase factor, we rewrite Eq. (12) as follows:

$$-[(N-1)/N]\varphi''(x)-(N-1)g\varphi^3(x)=\epsilon\,\varphi(x)\ . \qquad \text{(B6)}$$

Multiplying this equation by $\varphi'(x)$ and integrating we get

$$-[(N-1)/N][\varphi'(x)]^2-\tfrac{1}{2}(N-1)g\varphi^4(x)=\epsilon\varphi^2(x)\ . \qquad \text{(B7)}$$

To eliminate an additional integration constant in this equation we have again used the fact that both $\varphi(x)$ and $\varphi'(x)$ vanish asymptotically.

Equation (B7) can be rewritten as follows:

$$\varphi'(x)=\pm[N/(N-1)]^{1/2}\times\varphi(x)[-\epsilon-\tfrac{1}{2}(N-1)g\varphi^2(x)]^{1/2}, \qquad \text{(B8)}$$

and is clearly integrable by quadratures, yielding

$$\varphi(x)=\frac{\{-2\epsilon/[(N-1)g]\}^{1/2}}{\cosh\{[N/(N-1)]^{1/2}(-\epsilon)^{1/2}(x-a)\}}\ . \qquad \text{(B9)}$$

Here a is an arbitrary (integration) constant, whose presence corresponds to the translation-invariant nature of the problem.

There still remains to satisfy the normalization condition

$$\int_{-\infty}^{+\infty}dx[\varphi(x)]^2=1\ , \qquad \text{(B10)}$$

which, due to the nonlinearity of the problem, does play a nontrivial role. Indeed, inserting (B9) in (B10), there obtains the eigenvalue condition

$$\epsilon=\epsilon_{(N)}\ , \qquad \text{(B11)}$$

with $\epsilon_{(N)}$ given by Eq. (16).

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[1]One rigorous result concerns the coincidence of the exact and the Hartree-Fock values of the ground-state energy in the high-density limit [E. H. Lieb and M. De Llano, Phys. Lett. B 37, 47 (1971)]. Although this result is not applicable to the case considered here [because (i) it refers to the fermion case, (ii) the properties of the potential that are required for its validity do not hold in this case, and (iii) it refers to many-body systems included in a container, whose density can be increased *ad libitum* squeezing the container], it is consistent with the findings reported below.

[2]F. A. Berezin, G. P. Pochil, and V. M. Finkelberg, Moscow Univ. Vestnik 1, 21 (1964); J. B. McGuire, J. Math. Phys. 5, 622 (1964); E. Brezin and J. Zinn-Justin, C. R. Acad. Sci. (Paris) B263, 670 (1966); C. N. Yang, Phys. Rev. Lett. 19, 1312 (1967) and Phys. Rev. 168, 1920 (1968). Several recent papers extend this many-particle model and/or use it as a test case; but we have been unable to locate any paper using it to test the Hartree approximation.

[3]Units are chosen so that $\hbar^2/2m=1$, implying that g is an inverse length.

[4]This fact originates from the peculiar zero-range nature of the interaction; it contradicts a conjecture by E. Lieb and D. Mattis, *Mathematical Physics in One Dimension* (Academic, New York, 1966), p. 401 [see sentence after Eq. (5.26)].

[5]This wave function is now normalized to N upon integration over *all* the N coordinates x_i, without $\delta(x_{\text{c.m.}})$.

[6]The term $-g|\varphi(x)|^2$ corresponds of course to the Hartree effective potential $\int_{-\infty}^{+\infty}dx'\,v(x-x')\,|\varphi(x')|^2$, due to the δ-like nature of the two-body potential, $v(x)=-g\delta(x)$. In Eq. (12), and always in the following, primes stand for derivatives.

[7]Except for the (infinite) degeneracy originating from the translational invariance of (12) and corresponding to the arbitrariness implicit in the possibility to replace x by $x-a$, with a an arbitrary constant, on the right-hand side of (15) (see Appendix B).

[8]See, e.g., the review paper by F. Palumbo, in *The Nuclear Many-Body Problem*, edited by F. Calogero and C. Ciofi degli Atti (Editrice Compositori, Bologna, 1974), pp. 685–705.

[9]The exact coincidence of the differences between (20) and (17) and (17) and (9) is remarkable, but presumably of no significance.

[10]The factor N in this formula compensates the absence of a factor N^{-1} in the argument of the center-of-mass δ function in Eq. (A2).

[11]See, for instance, Eq. 2.1.5(30) in *Higher Transcendental Functions*, edited by A. Erdélyi (McGraw-Hill, New York, 1953), Vol. I, p. 66. To apply this formula to our case, set $a=1-N$, $n=m-1$, $c=b+2$ and take the limit $b\to+\infty$.

[12]Replace the summation index n by $k=N-1-n$, and then use the truncated binomial formula [see, for instance, Eq. (0.151.4)] in I. S. Gradshteyn and I. M. Ryzhik, *Tables of Integrals, Series and Products* (Academic, New York, 1965), p. 3.