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Analytical and numerical approximations to the delta interaction

R Alzetta and A M Pinna

Dipartimento di Fisica, Università della Calabria, Cosenza, Italy and CERN, Geneva, Switzerland

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Abstract. First-order perturbative corrections to the ground-state energy and Hartree-Fock equations are derived for the system of $(N+N)$ identical fermions attracted by a delta-function interaction on a circle of length L. Numerical results of Monte Carlo calculations for few fermions are presented and discussed.

1. Introduction

In a previous paper (Alzetta *et al* 1984) numerical results were presented from a simple lattice computer calculation for a one-dimensional system of few $(N+N)$ identical fermions, i.e. N of them 'spinning up' and N 'spinning down', mutually attracted by a delta interaction. The number N was confined there between 3 and 6, the lattice was small and coarse-grained, periodic boundary conditions (PBC) were introduced and the density (ρ) of fermions and the strength (g) of the interaction were kept constantly equal to one. Here we present numerical results using the same computational technique for two different classes of applications:

(i) smaller N ($N=1, 2, 3$), different fermion densities but same strength ($g=1$) of the delta interaction and same kind of states for the functional integral representation of the imaginary time evolution operator;

(ii) $N=5$, same fermion density ($\rho=1$) but different kind of representation of the evolution operator and various values of the strength of the interaction.

These latter applications allow the extension to our context of the variational method suggested by Wilson (1981) and applied, for example, by Falcioni *et al* (1982) and Berg *et al* (1982), and also allowed the calculation of the lowest excited-state energies in addition to the ground-state energy of the system. Furthermore the statistical method appears more efficient in these latter applications and ready for higher-dimensional more realistic cases.

Recent analogous Monte Carlo (MC) studies are those performed by Scalapino *et al* (1984) for a fermion lattice gas and by Hirsch and Scalapino (1984) in the framework of the Hubbard model. The numerical calculations are preceded by some elementary analytical results concerning first-order perturbative correction to the ground-state energy and the Hartree-Fock (HF) equation for the system of $(N+N)$ fermions with a two-body delta attraction among them, confined in a periodic one-dimensional interval.

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2. Perturbative correction to the energy

The Hamiltonian of $(N+N)$ particles mutually attracted by a delta-function potential in one dimension is the following:

$$H_{2N} = \sum_{k=1}^{2N} T_k - g \sum_{\substack{k=1 \\ (k<l)}}^{2N} \sum_{l=1}^{2N} \delta(x_k - x_l) \tag{1}$$

where $T = -\frac{1}{2} d^2/dx^2$ is the kinetic energy of the single particle (SP) and g is the strength of the interaction ($g > 0$). For simplicity units are defined such that $\hbar = m = 1$. The binding energy of the system of $(N+N)$ fermions is

$$B(N+N) = E_0^L(N+N) - E_0^\delta(N+N) \tag{2}$$

where $E_0^L(N+N)$ is the ground-state energy of $(N+N)$ free fermions and $E_0^\delta(N+N)$ is the corresponding energy of the mutually attracting fermions.

First-order perturbative correction, $B^{(1)}(N+N)$, to the free energy $E_0^L(N+N)$ is given by

$$B^{(1)}(N+N) = -\langle \psi_0(x_1, x_2, \ldots, x_{2N}) | V | \psi_0(x_1, x_2, \ldots, x_{2N}) \rangle \tag{3}$$

with

$$V = -g \sum_{\substack{k=1 \\ (k<l)}}^{2N} \sum_{l=1}^{2N} \delta(x_k - x_l) \tag{4}$$

and

$$\psi_0(x_1, x_2, \ldots, x_{2N}) = \frac{1}{N!} \det[\varphi_i(x_j)]_{i,j=1}^N \det[\varphi_k(x_{N+j})]_{k,j=1}^N \tag{5}$$

where $\det[\varphi_i(x_j)]_{i,j=1}^N$ is the determinantal wavefunction built with the lowest SP wavefunctions of the N particles. The SP wavefunctions are taken to be the real orthonormalised solutions of the SP free equation, which we write below in two different notations for the SP energies and SP eigenfunctions:

$$\begin{aligned} &T(x)\varphi_l(x) = \eta_l \varphi_l(x) && l = 1, 2, 3, \ldots \\ &T(x)u_n(x) = \varepsilon_n u_n(x) && n = 0, \pm 1, \pm 2, \ldots \end{aligned} \tag{6}$$

with PBC in a one-dimensional interval of length L:

$$\begin{aligned} &\varphi_1(x) = 1/\sqrt{L} = u_0(x) && \eta_1 = \varepsilon_0 = 0 \\ &\varphi_2(x) = (2/L)^{1/2} \cos k_L x = u_1(x) && \eta_2 = \varepsilon_1 = 2\pi^2/L^2 \\ &\varphi_3(x) = (2/L)^{1/2} \sin k_L x = u_{-1}(x) && \eta_3 = \varepsilon_{-1} = 2\pi^2/L^2 \\ &\varphi_4(x) = (2/L)^{1/2} \cos 2k_L x = u_2(x) && \eta_4 = \varepsilon_2 = 4(2\pi^2/L^2) \\ &\varphi_5(x) = (2/L)^{1/2} \sin 2k_L x = u_{-2}(x) && \eta_5 = \varepsilon_{-2} = 4(2\pi^2/L^2) \\ &\varphi_6(x) = (2/L)^{1/2} \cos 3k_L x = u_3(x) && \eta_6 = \varepsilon_3 = a(2\pi^2/L^2) \end{aligned} \tag{7}$$

where

$$k_L = 2\pi/L \qquad \varepsilon_n = n^2(2\pi^2/L^2) \qquad n = 0, \pm 1, \pm 2, \ldots \tag{8}$$

are the wavenumber quantum and the nth free SP energy in PBC, respectively. The relation between η_l and ε_n is the following:

$$\begin{aligned} &\eta_l = \varepsilon_{l/2} && \text{if } l \text{ is even} \\ &\eta_l = \varepsilon_{(l-1)/2} && \text{if } l \text{ is odd.} \end{aligned} \tag{9}$$

Thus we have

$$\begin{aligned} &E_0^L(N+N) = \frac{\pi^2}{3L^2}(N^2-1)N && \text{PBC, } N \text{ odd} \\ &E_0^L(N+N) = \frac{\pi^2}{3L^2}(N^2+2)N && \text{PBC, } N \text{ even} \end{aligned} \tag{10}$$

for N odd and N even, respectively, for the ground-state energy of the N free particles with PBC. For odd N the calculation of (3) is straightforward and gives

$$B^{(1)}(N+N) = g\sum_{k=1}^{N}\sum_{l=1}^{N}\int_0^L \mathrm{d}x\,\varphi_k^2(x)\varphi_l^2(x) = gN^2/L. \tag{11}$$

For even N the ground-state energy of the unperturbed system is four times degenerate. Therefore the solution of the secular equation gives four different values for $B^{(1)}(N+N)$. However, their average is the same as in (11) for odd N.

In conclusion the binding energy to first order is proportional to N^2, which is the number of all possible pairs of interacting particles (no saturation to this order) and is inversely proportional to the size L of the system.

3. The Hartree–Fock equation

If we calculate the expectation value $\langle H_{2N}\rangle$ of the Hamiltonian (1) in the state described by the determinantal wavefunction of type (5)

$$\psi_{N+N}(x_1, x_2, \ldots, x_{2N}) = \frac{1}{N!}\det[f_i(x_j)]_{i,j=1}^{N}\det[f_k(x_{N+j})]_{k,j=1}^{N} \tag{12}$$

where $f_i(x_j)$ is any orthonormalised set of SP wavefunctions satisfying PBC but not necessarily solutions of (6), we find

$$\langle\psi_{N+N}|H_{2N}|\psi_{N+N}\rangle = 2\sum_{l=1}^{N}\langle f_l|T|f_l\rangle - g\sum_{l=1}^{N}\sum_{k=1}^{N}\langle f_l f_k|\delta|f_l f_k\rangle \tag{13}$$

where

$$\langle f_l|T|f_l\rangle = -\frac{1}{2}\int_0^L f_l(x)\frac{\mathrm{d}^2}{\mathrm{d}x^2}f_l(x)\,\mathrm{d}x \tag{14}$$

and

$$\langle f_l f_k|\delta|f_l f_k\rangle = \int_0^L \mathrm{d}x_1\int_0^L \mathrm{d}x_2\, f_l(x_1)f_k(x_2)\delta(x_1-x_2)f_l(x_1)f_k(x_2) = \int_0^L \mathrm{d}x\, f_l^2(x)f_k^2(x). \tag{15}$$

Stationarity conditions

$$\delta\langle H_{2N}\rangle/\delta f_l = 0 \qquad l = 1, 2, \ldots, N$$

together with the normalisation constraint on the varied SP wavefunctions, then imply the following HF equation for the SP wavefunction of the system:

$$-\frac{1}{2}\frac{d^2}{dx^2}f_l(x) - g\sum_{k=1}^{N} f_k^2(x)f_l(x) = \varepsilon_l^{HF} f_l(x) \tag{16}$$

namely

$$(T + V^{HF}[f])f_l(x) = \varepsilon_l^{HF} f_l(x)$$

where

$$V^{HF}[f] = -g\sum_{k=1}^{N} f_k^2(x) \tag{17}$$

is the HF potential and ε_l^{HF} are the SP HF energies. The HF energy of the system of $(N+N)$ fermions will be

$$E_0^{HF}(N+N) = 2\sum_{l=1}^{N}\varepsilon_l^{HF} + g\sum_{l=1}^{N}\sum_{k=1}^{N}\int_0^L dx f_l^2(x)f_k^2(x). \tag{18}$$

The above formulae were already obtained by Lieb and de Llano (1978).

4. Numerical results: first part

We now present the numerical results for ground-state and binding energies for the cases $N = 1, 2, 3$, obtained by the same procedure used by Alzetta *et al* (1984) for the cases $N = 3, 4, 5, 6$. Eigenstates of the position operator are chosen as initial and final states of the matrix elements of the imaginary time evolution operator to obtain the functional integral representation of the few-particle propagator. For the free case

$$\begin{aligned} E_0^L(N) &= -\lim_{t\to\infty}\frac{1}{t}\ln G_N^L(\bar{y}^f, \bar{y}^i; t) \\ E_0^L(N+N) &= -\lim_{t\to\infty}\frac{1}{t}\ln G_{N+N}^L(\bar{y}^f, \bar{y}^i; t) \end{aligned} \tag{19}$$

where

$$G_N^L(\bar{y}^f, \bar{y}^i; t) = \det[G_1^L(y_a^f, y_b^i; t)]_{a,b=1}^N \tag{20a}$$

$$G_{N+N}^L(\bar{y}^f, \bar{y}^i; t) = \{\det[G_1^L(y_a^f, y_b^i; t)]_{a,b=1}^N\}^2 \tag{20b}$$

and

$$G_1^L(y_a^f, y_b^i; t) = \langle y_a^f|\exp(-tT)|y_b^i\rangle \tag{21}$$

is the SP propagator solution of the following free equation of motion:

$$\frac{\partial}{\partial t}G_1^L(x, y; t) = \frac{1}{2}\frac{\partial^2}{\partial x^2}G_1^L(x, y; t). \tag{22}$$

For the interacting case

$$E_0^\delta(N) = -\lim_{t\to\infty}\frac{1}{t}\ln G_N^\delta(\bar{y}^f, \bar{y}^i; t) \tag{23a}$$

$$E_0^\delta(N+N) = -\lim_{t\to\infty}\frac{1}{t}\ln G_{N+N}^\delta(\bar{y}^f, \bar{y}^i; t) \tag{23b}$$

where

$$G_N^\delta(\bar{y}^f, \bar{y}^i; t) = \int \mathrm{d}[A]\, p_\delta[A] \det[G_1^\delta(y_a^f, y_b^i; t|A)]_{a,b=1}^N \tag{24a}$$

$$G_{N+N}^\delta(\bar{y}^f, \bar{y}^i; t) = \int \mathrm{d}[A]\, p_\delta[A] \{\det[G_1^\delta(y_a^f, y_b^i; t|A)]_{a,b=1}^N\}^2 \tag{24b}$$

are the functional integral representations of the N particles and $(N+N)$ interacting-particle propagator, respectively. The SP propagator G_1^δ is a solution of the following equation of time evolution:

$$\begin{aligned} &\frac{\partial}{\partial t} G_1^\delta(x, y; t|A) = \left(\frac{1}{2}\frac{\partial^2}{\partial x^2} - A(x, t)\right) G_1^\delta(x, y; t|A) \\ &G_1^\delta(x, y; 0|A) = \delta(x-y) \end{aligned} \tag{25}$$

and $A(x, t)$ is the common random field with white-noise-type Gaussian distribution $p_\delta[A]$:

$$\begin{aligned} &p_\delta[A] = \exp\left(-\tfrac{1}{2}\int_0^t \mathrm{d}\tau \int \mathrm{d}x\, A^2(x, \tau)\right) \\ &\int \mathrm{d}[A]\, p_\delta[A] = 1. \end{aligned} \tag{26}$$

We will verify that

$$G_N^\delta(t) \simeq G_N^L(t) \qquad E_0^\delta(N) \simeq E_0^L(N) \tag{27}$$

as a consequence of the Pauli exclusion principle, i.e. the determinantal structure of the propagator.

The $L \times JT$ spacetime lattice for the MC calculations was taken fixed as far as the time spacing ($\varepsilon = 0.25$) and spatial spacing ($a = 1$) was concerned. Different values for ε ($\varepsilon = 0.125$, $\varepsilon = 0.5$) were tested and found uninteresting or inconvenient: the $\varepsilon = 0.125$ case uselessly removed the time asymptotic region further, whereas the $\varepsilon = 0.5$ case augmented the intensity of the random fluctuations of the results in the step concerning the numerical solution of the differential equation (25).

Different values for the length L, i.e. the number of space sites, were systematically taken in order to check the variation of the results with particle density $\rho = 2N/L$. A unit strength ($g = 1$) for the delta interaction has been introduced everywhere in this first part of our numerical calculations.

The results are summarised in table 1. The meaning of the various quantities present in table 1 is the following: N is the number of fermions of the same species, L is the length of space lattice, i.e. the number of space lattice sites, since $a = 1$. By ε we mean time lattice spacing, JT is the number of time lattice sites. $E_0^L(N)$ of column 5 is the ground-state energy of N free fermions of the same colour, analytically derived in three different cases.

(a) The ($a = 0$, $\varepsilon = 0$) case is the spacetime continuum case, in which SP energies are

$$\varepsilon_n(a = 0, \varepsilon = 0) = (2\pi^2/L^2)n^2 \qquad \text{PBC}, n = 0, \pm 1, \pm 2, \ldots. \tag{28}$$

(b) The ($a = 1$, $\varepsilon = 0$) case is the intermediate case of discrete-space continuous-time calculations, for which SP energies are

$$\varepsilon_n(a = 1, \varepsilon = 0) = 1 - \cos(2\pi n/L) \qquad \text{PBC}, n = 0, \pm 1, \pm 2, \ldots. \tag{29}$$

Table 1. Ground-state energies of N and $(N+n)$ free and delta-interacting fermions. The coupling constant $g=1$ everywhere. Time lattice spacing $\varepsilon=\frac{1}{4}$. Spatial spacing $a=1$. Representation of time evolution operator in terms of the particle propagator.

				$E_0^L(N)$				$E_0^L(N+N)$						
N	L	ε	JT	$a=0,\ \varepsilon=0$ $a=1,\ \varepsilon=0$ $a=1,\ \varepsilon$	$\Sigma_0^L(N)$ computer results	$\langle E_0^\delta(N)\rangle$	μ	$a=0,\ \varepsilon=0$ $a=1,\ \varepsilon=0$ $a=1,\ \varepsilon$	$E_0^L(N+N)$ computer results	$\langle E_0^\delta(N+N)\rangle$	μ	$B(N+N)$	NC	CPU on VAX 11/780
1	3	$\frac{1}{4}$	50	0 0 0	$<10^{-16}$	−0.0003	0.0005	0 0 0	$<10^{-16}$	−0.093	0.003	0.093	100 000	~$\frac{3}{4}$ h
1	4	$\frac{1}{4}$	50	0 0 0	$<10^{-16}$	0.0003	0.0004	0 0 0	0.3×10^{-11}	−0.068	0.002	0.068	100 000	~1 h
1	5	$\frac{1}{4}$	50	0 0 0	$<10^{-16}$	−0.0004	0.0004	0 0 0	0.3×10^{-7}	−0.055	0.002	0.055	100 000	~1.25 h
1	6	$\frac{1}{4}$	50	0 0 0	$<10^{-16}$	0.0004	0.0005	0 0 0	0.5×10^{-5}	−0.045	0.002	0.045	100 000	~1.5 h
1	7	$\frac{1}{4}$	50	0 0 0	$<10^{-16}$	−0.0002	0.0003	0 0 0	0.1×10^{-3}	−0.040	0.002	0.040	100 000	~1.75 h
1	8	$\frac{1}{4}$	50	0 0 0	$<10^{-16}$	0.0003	0.0006	0 0 0	0.8×10^{-3}	−0.031	0.002	0.031	100 000	~2 h
2	3	$\frac{1}{4}$	50	2.193 1.500 1.993	1.880	1.93	0.02	4.386 3.000 3.986	3.760	3.09	0.02	0.67	100 000	~1 h
2	4	$\frac{1}{4}$	50	1.234 1.000 1.170	1.151	1.149	0.005	2.467 2.000 2.341	2.301	1.860	0.004	0.441	50 000	~$\frac{3}{4}$ h
2	6	$\frac{1}{4}$	50	0.548 0.500 0.536	0.534	0.539	0.005	1.097 1.000 1.068	1.068	0.811	0.015	0.257	50 000	~1.25 h
2	8	$\frac{1}{4}$	50	0.308 0.293 0.305	0.304	0.304	0.002	0.617 0.586 0.609	0.608	0.404	0.011	0.204	50 000	~2 h
3	3	$\frac{1}{4}$	30	4.387 3.000 3.986	3.760	3.756	0.005	8.773 6.000 7.971	7.520	6.11	0.03	1.41	100 000	~$\frac{3}{4}$ h
3	6	$\frac{1}{4}$	50	1.097 1.000 1.075	1.068	1.059	0.006	2.193 2.000 2.150	2.136	1.68	0.05	0.46	20 000	~1 h
3	12	$\frac{1}{4}$	50	0.274 0.268 0.272	0.273	0.254	0.006	0.548 0.536 0.544	0.545	0.42	0.02	0.13	20 000	~8 h

(c) The $(a=1, \varepsilon)$ case comes from the SP spacetime lattice spectrum, analytically approximated by taking into account the effect of the finite size of spacetime lattice spacing on SP energies in the spacetime continuum:

$$\varepsilon_n(a=1, \varepsilon) \simeq \varepsilon_n(a=0, \varepsilon=0) + \tfrac{1}{2}(\varepsilon - \tfrac{1}{3})\varepsilon_n^2(a=0, \varepsilon=0) \tag{30}$$

(the above formula is valid for small values of n only, see (52) of Alzetta *et al* (1984)).

The values $E_0^L(N)$ in the sixth column are numerical results of our computer calculation. The procedure which leads to them is widely explained in § 4 of Alzetta *et al* (1984). We here summarise the main lines of the procedure: we first introduced a $L \times JT$ spacetime lattice with L spatial sites of length $a=1$ and JT time sites of length $\varepsilon = 0.25$, imposed periodicity on the space component and solved equation (22) numerically for the free particle. Then we calculated, for JT different values of time, the Green function for N free indistinguishable fermions, i.e. the determinant of $(20a)$. The final results appeared independent of the choice of the initial state configuration $\bar{y}^i$; as far as final states are concerned we did not choose any particular state, since we calculated instead the sum of all G_N^L with different possible final states $\bar{y}^f$ consistent with the Pauli principle. The advantage of such a summation was that it delocalised the final state of the system consequently anticipating, by the uncertainty principle, the time asymptotic exponential region for the Green function, necessary to extract, by means of (19), the energy of the ground state.

The quantities $\langle E_0^\delta(N)\rangle$ in column 7 of table 1 are MC averages of the ground-state energies of N indistinguishable fermions among which a delta potential is present but actually ineffective as it is manifest in the results showing only negligible discrepancies with free case $E_0^L(N)$. The terms μ in column 8 indicate the standard errors of the preceding averages $\langle E_0^\delta(N)\rangle$ listed in column 7. Columns 7 and 8 contain the first significant results of our numerical experiment and should be used as a check of our statistical accuracy.

In columns 9-12 the corresponding values for the $(N+N)$ system are presented. In order to obtain the computer results of column 10 of table 1, the same procedure which yields column 6 was carried out, with the only difference being squaring the Slater determinant in order to obtain, by $(20b)$, the Green function of $(N+N)$ free fermions of two species. The numerical results listed in columns 7 and 11 of table 1 are obtained by substituting (23)-(25) to (19)-(22) in the numerical procedure previously explained for the free case. The random common field $A(x, t)$ of (25) was simulated by extracting from the computer a finite but large and discrete Gaussian distribution of random lattice fields $A(x_i, t_j)$ $(i=1, 2, \ldots, L; j=1, 2, \ldots, JT)$. We have called NC, and listed in column 14 of table 1 as the number of MC sweeps, the number of such random fields which have been constructed by assigning each point of the spacetime lattice NC random numbers in a numerically approximated Gaussian distribution with zero mean and unit standard deviation.

The last three columns (13-15) indicate the binding energy:

$$B(N+N) = E_0^L(N+N) - \langle E_0^\delta(N+N)\rangle \tag{31}$$

the number NC of MC sweeps and finally the CPU time spent on a VAX 11/780.

We postpone to § 6 comments and discussion on the above results and their comparison with those results on the same problem already present in the literature. We want here to comment on one single point only: the result listed in row 13 of table 1 ($N=3$, $L=6$, $\varepsilon=0.25$, $JT=50$), if compared with the corresponding results previously obtained by Alzetta *et al* (1984), shows a considerable discrepancy in the most

interesting values $E_0^{\delta}(3+3)$ and $B(3+3)$: 1.68 and 0.46, respectively, against 1.85 and 0.29 of that paper. These discrepancies, which are beyond statistical errors μ (0.05 and 0.06, respectively), are probably due to the previous too poor statistics (only 3000 MC sweeps) used in the earlier work.

5. Numerical results: second part

In the second part of our numerical experiment on delta-function interaction, we changed the states of the representation of the time-evolution operator: instead of looking for the functional integral representation of the N- and $(N+N)$-particle propagator, we built up the representation of the imaginary time evolution operator into the space of eigenstates of the energy of N and $(N+N)$ free particles. The following quantity:

$$R_{\beta\alpha}(t) = \langle\beta| \exp(-tH_N)|\alpha\rangle \tag{32}$$

represents the matrix element of the imaginary time evolution operator of N fermions calculated between two eigenstates of the energy of N free indistinguishable fermions, i.e. between two Slater determinants built with N different eigenfunctions of type (7). We use the following notation for the main formulae:

$$\begin{aligned} R_{\beta\alpha}(t) &= \langle\beta| \exp(-tH_N)|\alpha\rangle \\ &= \langle \det[F_{l,m}(t|A)]_{l,m=1}^{N} \rangle_{p_\delta} \\ &= \int \mathrm{d}[A]\, p_\delta[A] \det[F_{l,m}(t|A)]_{l,m=1}^{N} \end{aligned} \tag{33}$$

where

$$\begin{aligned} F_{l,m}(t|A) &= \langle\varphi_l|\exp(-th_1[A])|\varphi_m\rangle \\ &= \int_0^L \mathrm{d}x\, \varphi_l(x) \exp[-th_1(x|A)]\varphi_m(x) \end{aligned} \tag{34}$$

is the SP Green function satisfying the following initial condition:

$$F_{l,m}(0|A) = \delta_{l,m}. \tag{35}$$

The following wavefunction:

$$f_m(x;\, t|A) = \exp[-th_1(x|A)]\varphi_m(x)$$

is the solution of the same differential equation (25) satisfied by the SP propagator G_1^{δ}:

$$\frac{\partial}{\partial t} f_m(x;\, t|A) = \left(\frac{1}{2}\frac{\partial^2}{\partial x^2} - A(x,\, t)\right) f_m(x;\, t|A). \tag{36}$$

The φ are defined in (7) and

$$h_1(x|A) = -\frac{1}{2}\frac{\partial^2}{\partial x^2} + A(x,\, t). \tag{37}$$

$A(x,\, t)$ is the common random field and l and m run over all SP quantum numbers present in the N-particle states β and α, respectively.

For the $(N+N)$-particle system we have simply to square determinants. The matrix $R(t)$ in (32), as well as the following matrix:

$$RR(t) = \langle \{\det[F_{l,m}(t|A)]_{l,m=1}^{N}\}^2 \rangle_{p_\delta} \tag{38}$$

are $NS \times NS$ matrices, where NS is the dimension of the truncated space of N-fermion states, namely the number of different N-fermion states we introduced in the calculations. We verified that with this second choice of initial and final states the time asymptotic region for (19) and (23) was immediately reached at the second or third time step of the computer calculations, instead of after nearly ten steps of the first, propagator, case, with a consequent saving of computer time.

In order to correct for the effect of the truncation of the set of N-particle states, we adopted the Wilson variational procedure used by Falcioni *et al* (1982) and Berg *et al* (1982). We define the following $NS \times NS$ matrices:

$$C(n) = R(t = n\varepsilon) \qquad CC(n) = RR(t = n\varepsilon) \qquad n = 0, 1, 2, \ldots, JT-1 \tag{39}$$

and then construct the following $NS \times NS$ matrices:

$$\begin{aligned} &CT(n) = [C(n-1)]^{-1/2} C(n) [C(n-1)]^{-1/2} \\ &CCT(n) = [CC(n-1)]^{-1/2} CC(n) [CC(n-1)]^{-1/2} \qquad n = 1, 2, 3, \ldots, JT-1 \end{aligned} \tag{40a}$$

and

$$\begin{aligned} &CF(n) = C(n-1)[C(n-2)]^{-1} C(n-1) \\ &CCF(n) = CC(n-1)[CC(n-2)]^{-1} CC(n-1) \qquad n = 3, 4, \ldots, JT-1. \end{aligned} \tag{40b}$$

Inside a non-truncated state space ($NS = \infty$) we would have exactly

$$CT(n) = C(1) \qquad CCT(n) = CC(1) \qquad n = 1, 2, 3, \ldots, JT-1 \tag{41}$$

and

$$CF(n) = C(n) \qquad CCF(n) = CC(n) \qquad n = 3, 4, 5, \ldots, JT-1. \tag{42}$$

In our truncated NS-state space ($NS = 5$-8) we will have approximately results (41), and (42) will work as a consistency check of the approach at higher times.

Diagonalising matrices (40) into the space of NS lowest N-particle states, one will obtain the lower part of the spectrum of the N-particle and $(N+N)$-particle system. Calling $\eta t(n)$ and $\eta\eta t(n)$ $(n = 1, 2, \ldots, JT-1)$ any one of the NS eigenvalues of the $2 \times (JT-1)$ matrices (40a), we will be authorised to write

$$\begin{aligned} &E^\delta(N) \simeq -(1/\varepsilon) \ln \eta t(n) \\ &E^\delta(N+N) \simeq -(1/\varepsilon) \ln \eta\eta t(n) \qquad n = 1, 2, 3, \ldots, JT-1 \end{aligned} \tag{43}$$

for the lowest energy levels of N fermions and $(N+N)$ fermions, respectively.

In table 2 we summarise the results of our numerical experiment for the system of five fermions of the same species. Each of the seven energy levels reported in columns 3, 5, 7, 9, 11, 13 and 15 is the average, for a different value of g in each column, of the $JT-1$ energies extracted from the eigenvalues of $CT(n)$ matrices ($n = 1, 2, \ldots, JT-1$) by means of (43) and each σ value beside it on the right-hand side is the standard deviation from that average of those $JT-1$ energies. The number JT of time steps was equal to 8 or 7. The length L of the spatial periodic interval was kept constant and equal to ten ($\rho = 1$). A time lattice spacing $\varepsilon = \frac{1}{8}$ was chosen. NS is 7; in fact, we list seven energy levels. However, results appeared insensitive to small variations (5-8)

Table 2. Lowest energy levels of the system of five indistinguishable fermions, free and delta interacting. $L = 10$, $\epsilon = \frac{1}{8}$, $NS = 7$:

$$\sigma_N^2 = \frac{1}{N}\sum_{i=1}^{N}(E_k^{(i)}(5) - \langle E_k(5)\rangle)^2 \qquad k = 1, 2, \ldots, 7.$$

Seven five-fermion states in I notation of (7): $|1\rangle = (1, 2, 3, 4, 5)$; $|2\rangle = (1, 2, 3, 4, 6)$; $|3\rangle = (1, 2, 4, 5, 6)$; $|4\rangle = (1, 2, 3, 6, 7)$; $|5\rangle = (2, 3, 4, 5, 6)$; $|6\rangle = (1, 2, 3, 6, 8)$; $|7\rangle = (1, 4, 5, 6, 7)$. Representation of time evolution operator into the space of NS five-free-particle-energy eigenstates.

		$g = 1$		$g = 2$		$g = 3$		$g = 4$		$g = 5$		$g = 6$		$g = 10$	
	Free fermions	$NC =$ 1000	σ_7	$NC =$ 2000	σ_7	$NC =$ 3000	σ_6	$NC =$ 4000	σ_6	$NC =$ 5000	σ_6	$NC =$ 6000	σ_6	$NC =$ 10 000	σ_6
$\langle E_7(5)\rangle$	4.304	4.298	0.057	4.325	0.066	4.342	0.050	4.282	0.053	4.258	0.122	4.229	0.114	4.253	0.083
$\langle E_6(5)\rangle$	3.867	3.932	0.047	3.849	0.057	3.823	0.057	3.904	0.088	3.885	0.106	3.917	0.034	3.928	0.059
$\langle E_5(5)\rangle$	3.261	3.300	0.036	3.270	0.054	3.288	0.034	3.296	0.028	3.336	0.040	3.311	0.066	3.300	0.088
$\langle E_4(5)\rangle$	3.246	3.264	0.059	3.220	0.029	3.201	0.043	3.222	0.031	3.239	0.083	3.213	0.095	3.216	0.047
$\langle E_3(5)\rangle$	3.068	3.088	0.031	3.062	0.062	3.066	0.053	3.079	0.086	3.058	0.040	3.104	0.092	3.093	0.100
$\langle E_2(5)\rangle$	2.539	2.523	0.048	2.526	0.043	2.580	0.062	2.566	0.062	2.551	0.103	2.583	0.136	2.536	0.054
$\langle E_1(5)\rangle$	1.832	1.830	0.037	1.837	0.050	1.834	0.033	1.819	0.032	1.814	0.024	1.816	0.030	1.854	0.084
$\langle\sigma\rangle$			0.05		0.05		0.05		0.05		0.07		0.08		0.07
CPU on VAX 11/780	9 s	1.5 h		3 h		4.5 h		6 h		7.5 h		9 h		13 h	
JT	8	8		8		8		8		8		8		7	

Table 3. Lowest energy levels of (5+5) free and delta-interacting fermions. $L = 10$, $\varepsilon = \frac{1}{8}$, $NS = 7$, $\rho = 1$.

		$g = 1$			$g = 2$			$g = 3$			$g = 4$			$g = 5$			$g = 6$			$g = 10$		
	Free fermions	$NC =$ 1000	B	σ_7	$NC =$ 2000	B	σ_7	$NC =$ 3000	B	σ_6	$NC =$ 4000	B	σ_6	$NC =$ 5000	B	σ_6	$NC =$ 6000	B	σ_6	$NC =$ 10 000	B	σ_6
$\langle E_7(5+5)\rangle$	8.608	8.230	0.378	0.140	7.925	0.684	0.164	7.579	1.030	0.146	6.791	1.817	0.508	6.200	2.409	0.567	6.283	2.325	0.132	4.989	3.619	0.484
$\langle E_6(5+5)\rangle$	7.734	7.483	0.251	0.147	6.863	0.871	0.231	6.298	1.436	0.346	6.257	1.476	0.249	5.671	2.063	0.268	5.513	2.220	0.314	4.046	3.688	0.305
$\langle E_5(5+5)\rangle$	6.523	6.261	0.262	0.099	5.866	0.657	0.276	5.504	1.019	0.071	5.240	1.283	0.294	4.965	1.557	0.091	4.654	1.869	0.576	3.117	3.406	0.545
$\langle E_4(5+5)\rangle$	6.491	6.140	0.351	0.106	5.680	0.812	0.160	5.308	1.183	0.134	4.956	1.535	0.195	4.621	1.870	0.241	4.269	2.222	0.411	2.817	3.674	0.426
$\langle E_3(5+5)\rangle$	6.136	5.788	0.348	0.063	5.303	0.833	0.187	4.982	1.154	0.165	4.652	1.484	0.294	4.381	1.755	0.175	3.773	2.363	0.430	2.513	3.623	0.506
$\langle E_2(5+5)\rangle$	5.077	4.608	0.469	0.164	4.295	0.783	0.114	4.013	1.064	0.092	3.577	1.561	0.188	3.246	1.832	0.336	2.961	2.116	0.519	1.263	3.815	0.863
$\langle E_1(5+5)\rangle$	3.664	3.285	0.379	0.123	2.966	0.698	0.178	2.642	1.022	0.164	2.285	1.379	0.215	2.009	1.655	0.243	1.727	1.937	0.309	0.460	3.204	0.682
			0.35	0.12		0.76	0.19		1.13	0.16		1.50	0.28		1.88	0.27		2.15	0.38		3.58	0.540
$\sigma(B)$			0.07			0.08			0.14			0.15			0.26			0.17			0.19	
CPU	9 s	1.5 h			3 h			4.5 h			6 h			7.5 h			9 h			13 h		
$\langle B\rangle/g$		0.35			0.38			0.38			0.38			0.38			0.36			0.36		

of *NS*. Different strengths g ($g = 1, 2, 3, 4, 5, 6$ and 10) for the delta force were taken which forced us to raise proportionally, from 1000 to 10 000, the number NC of MC sweeps to keep the fluctuations of the results nearly constant, as is manifest from the ninth row of table 2 which shows the average values $\langle\sigma\rangle$ of the standard deviations of the energies listed above them. The seven five-fermion states were chosen as follows, in the l-quantum number notation of (7):

$$\begin{aligned}
|1\rangle &= (1, 2, 3, 4, 5) \\
|2\rangle &= (1, 2, 3, 4, 6) \\
|3\rangle &= (1, 2, 4, 5, 6) \\
|4\rangle &= (1, 2, 3, 6, 7) \\
|5\rangle &= (2, 3, 4, 5, 6) \\
|6\rangle &= (1, 2, 3, 6, 8) \\
|7\rangle &= (1, 4, 5, 6, 7).
\end{aligned} \tag{44}$$

A comparison of the results obtained by MC simulation of the delta interaction reported in columns 3, 5, 7, 9, 11, 13 and 15 with the results of the computer calculation for free fermions, reported in column 2 of the same table 2, confirms the statistical accuracy of our calculations.

In table 3 we report the corresponding results for the case of the system of $(5+5)$ fermions. In row 9 the average values are reported of the numbers listed above them in the same column. In row 10 we list the standard deviations $\sigma(B)$ from the mean value $\langle B\rangle$ of the binding energies reported in the same column.

6. Discussion of results

(a) The average value of the binding energy for $(5+5)$ particles with $g = 1$ reported in table 3:

$$\langle B(5+5)\rangle = 0.35 \pm 0.03 \tag{45}$$

agrees with the result ($B_5 = 0.38$) previously obtained by Alzetta *et al* (1984) with the first method.

(b) For g different from one, the numbers listed in the twelfth row of table 3 suggest that the binding energy is proportional to the coupling constant:

$$B(N+N) \propto g \tag{46}$$

at least for small g.

(c) For $N = 1$ a least-squares fit has been made of the L dependence of the binding energy $B(1+1)$ reported in table 1: the result is the following:

$$B(1+1, L) = d/L \tag{47}$$

with $d = 0.274 \pm 0.012$ ($g = 1$).

Let us recall that the energy of the bound state of a pair of identical but distinguishable particles attracted by a delta potential for open (i.e. no wall of any kind to contain the particles) boundary conditions (density $\rho = 0$) was calculated by McGuire (1966) and found to be

$$E_0^{\delta}(1+1) = -g^2/4. \tag{48}$$

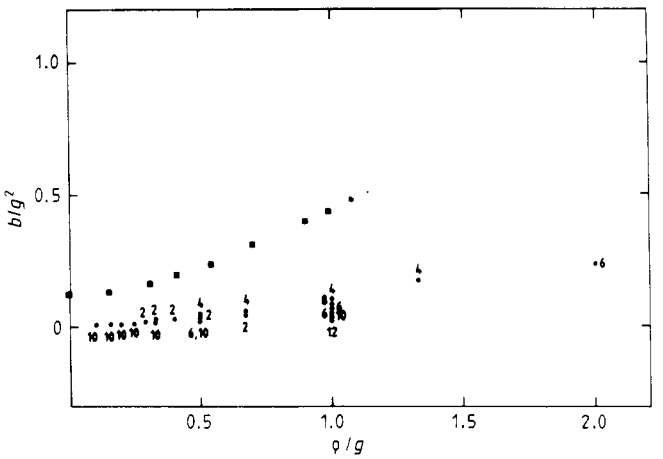

Figure 1. Binding energy per particle divided by the square of the strength of the delta force, b/g^2, plotted against density per unit coupling, ρ/g; $\rho = 2N/L$. ■ refers to values from Aguilera-Navarro *et al* (1982), while ● refers to the present work and to the earlier paper by Alzetta *et al* (1984). Small numbers near points indicate the total number of fermions $2N$. $b = B(N+N)/2N$.

Now if we apply to (47) our conjecture (46), we would have the following L and g dependence of $B(1+1)$:

$$B(1+1, L, g) = (d/L)g. \tag{49}$$

Comparison of (49) with (48) suggests that L works like $1/g$ for large systems (scaling property, see Lieb and de Llano (1978)).

(d) In figure 1 we compare our numerical results, together with those of the previous paper (Alzetta *et al* 1984), with the values produced by Aguilera *et al* (1982) by solving numerically the Gaudin equations which give the exact ground-state energy per particle, $\varepsilon(\rho) = E_0^{\delta}(N+N)/2N$, for any value of the density $\rho = 2N/L$ of the system. Figure 1 shows the numerical values b/g^2 of the binding energy per particle b divided by the square of the coupling constant g plotted against ρ/g, namely the density ρ per unit coupling. Square points refer to the values extracted from the results reported by Aguilera *et al* (1982), while round points refer to this work and the earlier paper. The above comparison, however, is rather far from being significant because, while we use small numbers N of fermions in periodic boundary conditions, all those numbers, as well as all others produced by various authors and reported by Aguilera *et al* (1982), are given in the limit of large system (Lieb and Liniger 1963, Gaudin 1967) or in the thermodynamic limit (Overhauser 1960, de Llano and Plastino 1976, Döhnert *et al* 1978, Gutierrez and Plastino 1981).

(e) From figure 1 one can appreciate the rather good agreement of our results for the same ρ/g but different values of N, even before the thermodynamic limit.

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