IFUSP/P-119

APPROXIMATE SOLUTIONS FOR GENERAL PAIRING HAMILTONIAN BY VARIATIONAL METHOD

by

A. Kamimura
Departamento de Física Nuclear, Instituto de Física
Universidade de São Paulo, São Paulo, S.P., Brasil.

APPROXIMATE SOLUTIONS FOR GENERAL PAIRING HAMILTONIAN BY VARIATIONAL METHOD

A. Kamimura

Departamento de Física Nuclear, Instituto de Física - U.S.P.

São Paulo, SP, Brasil

ABSTRACT

We present here, as a simple exercise of Quantum Mechanics, a method to calculate states of seniority zero of a general pairing Hamiltonian within the approximation where the matrix elements $g_{jj'}$ are not far from an average value $\bar{g}$. The set of coupled equations reduces to that obtained by Richardson[1], when all $g_{ij}=g$. Calculations for simple systems for one and two pairs are presented too.

The study of exact eigenstates with constant pairing-force Hamiltonian using non-quasiparticles methods was developed some years ago by R.Richardson et al[1]. They assume a many-fermion system contained in a fixed external potential well interacting via pairing forces and they denote by $(f\sigma)$ the single particle quantum numbers, ε_f the single-particle energy levels of this potential well and $\sigma=\pm$ denotes states wich are conjugate with respect to time reversal.

The Hamiltonian is written as

$$H_p = \sum_f 2\varepsilon_f \hat{N}_f - g\sum_f \sum_{f'} b_f^+ b_{f'} \tag{1}$$

where
$$\hat{N}_f = \frac{1}{2}\left(a_{f+}^+ a_{f+} + a_{f-}^+ a_{f-}\right) \tag{1-a}$$

$$b_f = a_{f-} a_{f+} \tag{1-b}$$

$a_{f\sigma}^+$, $(a_{f\sigma})$ are fermion creation (annihilation) operators satisfying anticommutation relations and the b's the following commutation relations:

$$\left[b_f, b_{f'}^+\right] = \delta_{ff'}\left(1-2\hat{N}_f\right) \tag{2-a}$$

$$\left[b_f, \hat{N}_{f'}\right] = \delta_{ff'} b_f \tag{2-b}$$

The exact eigenstates of N pairs of particles coupled to J=0 being of the form:

$$|\psi\rangle = \frac{1}{\sqrt{N!}} \sum_{f_1 \cdots f_N} \psi(f_1 \cdots f_N)\, b_{f_1}^+ \cdots b_{f_N}^+ |0\rangle \tag{3}$$

where $$\psi(f_1 \cdots f_N) = S^{(f)} \left\{ \prod_{k=1}^{N} (2\varepsilon_{f_k} - E_{p_k})^{-1} \right\} \tag{3-a}$$

$|0\rangle$ = real vacuum

and $S^{(f)}$ is the symmetrizer operator, i.e., the sum of all operators of permutation group S_N, applied in (f_j) space, in order to symmetrize the wave function. The total energy

$$E = E_{p_1} + E_{p_2} + \cdots E_{p_N} = \sum_{i=1}^{N} E_{p_i} \tag{4}$$

is obtained by solving the set of N coupled equations for the E_{p_i}

$$\frac{1}{g} + \sum_{j} \frac{2}{E_{p_j} - E_{p_i}} - \sum_{f'} \frac{1}{2\varepsilon_{f'} - E_{p_i}} = 0 \tag{5}$$

$i = 1, 2 \ldots N$ and $j \neq i$

Now, using variational technics, we intend to solve a more general Hamiltonian, keeping the form of wave function (3) and the Hamiltonian with f-dependent matrix elements, written as:

$$H = \sum_{f} 2\varepsilon_f \hat{N}_f - \sum_{f} \sum_{f'} g_{ff'} b_f^+ b_{f'} \tag{6}$$

Applying the variational method[2] we have

$$\delta E[\psi] = 0 \tag{7}$$

where $$E[\psi] = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} \tag{8}$$

or (7) can the replaced by:

$$\langle\delta\psi|(H - E)|\psi\rangle = 0 \tag{9}$$

with $$\langle \psi | \psi \rangle \neq 0 \tag{10}$$

and the variation is made over the complex parameters E_{pi}^* . If we have obtained the correct wave functions such that the condition (7) is fulfilled, we can calculate the energy by formula (8), wich can be evaluated as,

$$E = \sum_{i=1}^{N} E_{pi} + \Delta(E_{p1} \ldots E_{pN}) \tag{11}$$

and

$$\Delta(E_{p1} \ldots E_{pN}) = \sum_{f_1 \ldots f_N} \sum_{k} \left\{ \prod_{\sigma \neq k} \frac{1}{(2\mathcal{E}_{f\sigma} - E_{p\sigma})} S^{(f)} \left[\prod_{\sigma} \frac{1}{(2\mathcal{E}_{f\sigma} - E_{p\sigma}^*)} \left(1 + \sum_{l} \frac{2 g_{f_l f_k}}{E_{pl} - E_{pk}} - \sum_{f} \frac{g_{f_k f}}{2\mathcal{E}_f - E_{pk}} \right) \right] \right\} \Big/ \sum_{f_1 \ldots f_N} \left[\prod_{\sigma} \frac{1}{(2\mathcal{E}_{f\sigma} - E_{p\sigma})} S^{(f)} \left(\prod_{\sigma'} \frac{1}{(2\mathcal{E}_{f\sigma'} - E_{p\sigma'})} \right) \right] \tag{12}$$

Examining equation (12) we see that if all the g_{ij} are equal, Δ becomes zero since in this case prevail eq.(5), and equations (11) and (4) becomes the same, as expected. Then if we have each of the matrix element g_{ij} not far from the average value of $g_{ij} = \overline{g_{ij}}$, we expect that Δ is small and do not vary in a appreciable way as a function of parameters E_{pi}^* : With this approximation we change E of equation (9) by $\sum_i E_{pi}$ and performing variation over the parameters E_{pi}^* , we end with the following set of N coupled equations,

$$\sum_{f_1 \ldots f_N} \sum_{i}^{N} \left\{ \left(\prod_{\sigma \neq i} \frac{1}{(2\mathcal{E}_{f\sigma} - E_{p\sigma})} \right) \left\{ S^{(f)} \left(\prod_{\lambda} \frac{1}{(2\mathcal{E}_{f\sigma} - E_{p\lambda}^*)} \cdot \frac{1}{(2\mathcal{E}_{f\nu} - E_{p\nu}^*)} \right) \right\} \times \left[1 + \sum_{k \neq i} \frac{2 g_{f_k f_i}}{E_{pk} - E_{pi}} - \sum_{j} \frac{g_{f_i f_j}}{2\mathcal{E}_{fj} - E_{pi}} \right] \right\} + \chi_\nu\left(\Delta, \frac{\partial \Delta}{\partial E_{pi}^*} \ldots, E_{p1} \ldots, E_{p1}^* \ldots\right) = 0 \tag{13}$$

$\nu = 1 \ldots N$

After solving this set of equations we can get the total energy by formula (4) or by (11) calculating the small correction Δ (a posteriori) by equation (12).

The wave functions can be obtained through formula (3). Clearly we have to exclude from (13), the roots going to $\pm\infty$ for this corresponds to wave functions wich doesn't satisfy condition (10).

It is clear that, to solve the set of equations (13) can be more complicated than diagonalize the correspondent problem and get the exact solution. Then, for practical purposes (when the g_{ij} are not for from a cte value, and consequently $\Delta \sim 0$) we neglect in (13) the complicated function χ_ν, that is proportional to Δ and derivatives of Δ. Within this same spirit we eliminate the sum over $\underline{i}$ in (13) and we get a more simple set of equations:

$$\sum_{f_1 \ldots f_N} \left\{ \left[\prod_{\sigma \neq \nu} \frac{1}{(2\epsilon_{f\sigma} - E_{p\sigma})} \right] \left\{ S^{(f)} \cdot \left[\prod_{\lambda} \frac{1}{(2\epsilon_{f\lambda} - E^*_{p\lambda})} \cdot \frac{1}{(2\epsilon_{f\nu} - E^*_{p\nu})} \right] \right\}^* \cdot \left[1 + \right.\right.$$

$$\left. + \sum_{k \neq \nu} \frac{2 g_{f_k f_\nu}}{E_{pk} - E_{p\nu}} - \sum_j \frac{g_{f_\nu f_j}}{2\epsilon_{f_j} - E_{p\nu}} \right] = 0 \qquad (14)$$

$$\nu = 1 \ldots N$$

<u>Two illustrative examples: the one and two pairs systems.</u>

For N=1, equation (13) is

$$\sum_f \frac{1}{(2\epsilon_f - E^*_p)^2} \left[1 - \sum_{f'} \frac{g_{ff'}}{2\epsilon_{f'} - E_p} \right] - \chi_1 (\Delta, E^*_p, \epsilon_p) = 0 \qquad (15)$$

$$\Delta = \frac{\sum_{f'} \frac{1}{(2\varepsilon_{f'} - E_p^*)} \left(1 - \sum_{f} \frac{g_{ff'}}{2\varepsilon_f - E_p}\right)}{\sum_{f} \frac{1}{(2\varepsilon_f - E_p^*)(2\varepsilon_f - E_p)}} \tag{16}$$

$$E = E_p + \Delta \tag{17}$$

$$\chi_1 \simeq \sum_{f} \frac{\Delta}{(2\varepsilon_f - E_p^*)^2 (2\varepsilon_f - E_p)} \tag{17'}$$

where the sign $\simeq$ means that we neglect the derivative of Δ respect to E_p^*.

Note that if $g_{ff'}=g$, we have the well known exact solution[1]:

$$\frac{1}{g} = \sum_{f'} \frac{1}{(2\varepsilon_{f'} - E_e)} \tag{16'}$$

with $\Delta = 0$ and $\chi_1 = 0$.

For N=2, we have, by eq.(13)

$$1)\ \left[\sum_{f_1 f_2} \frac{1}{(f_1 - E_{p2})} \left(\frac{1}{(f_2 - E_{p1}^*)^2 (f_1 - E_{p2}^*)} + \frac{1}{(f_1 - E_{p1}^*)^2 (f_2 - E_{p2}^*)}\right)\left(1 - \sum_{f'} \frac{g_{ff'}}{(f' - E_{p1})} - \frac{2 g_{f_1 f_2}}{(E_{p1} - E_{p2})}\right)\right] + \left[\sum_{f_1 f_2} \frac{1}{(f_1 - E_{p1})} \left(\frac{1}{(f_1 - E_{p1}^*)^2 (f_2 - E_{p2}^*)} + \frac{1}{(f_2 - E_{p1}^*)^2 (f_1 - E_{p2}^*)}\right)\left(1 - \sum_{f'} \frac{g_{ff'}}{(f' - E_{p2})} + \frac{2 g_{f_1 f_2}}{(E_{p1} - E_{p2})}\right)\right] + \chi_1(\Delta, \ldots) = 0 \tag{18}$$

and

$$2)\left[\sum_{f_1f_2}\frac{1}{(f_1-E_{p_2})}\left(\frac{1}{(f_2-E^*_{p_1})(f_1-E^*_{p_2})^2}+\frac{1}{(f_1-E^*_{p_1})(f_2-E^*_{p_2})^2}\right)\left(1-\sum_{f'}\frac{g_{ff'}}{(f'-E_{p_1})}-\frac{2g_{f_1f_2}}{(E_{p_1}-E_{p_2})}\right)\right]+\left[\sum_{f_1f_2}\frac{1}{(f_1-E_{p_1})}\left(\frac{1}{(f_1-E^*_{p_1})(f_2-E^*_{p_2})^2}+\frac{1}{(f_2-E^*_{p_1})(f_1-E^*_{p_2})^2}\right)\times\right.$$

$$\left.\times\left(1-\sum_{f'}\frac{g_{ff'}}{(f'-E_{p_2})}+\frac{2g_{f_1f_2}}{(E_{p_1}-E_{p_2})}\right)\right]+\chi_2(\Delta,\dots)=0 \qquad (19)$$

and

$$\Delta=\left\{\sum_{f_1f_2}\frac{1}{(f_1-E_{p_2})}\left[\frac{1}{(f_2-E^*_{p_1})(f_1-E^*_{p_2})}+\frac{1}{(f_1-E^*_{p_1})(f_2-E^*_{p_2})}\right]\left[1-\sum_{f'}\frac{g_{ff'}}{(f'-E_{p_1})}-\frac{2g_{f_1f_2}}{(E_{p_1}-E_{p_2})}\right]+\right.$$

$$\left.+\sum_{f_1f_2}\frac{1}{(f_1-E_{p_1})}\left[\frac{1}{(f_1-E^*_{p_1})(f_2-E^*_{p_2})}+\frac{1}{(f_2-E^*_{p_1})(f_1-E^*_{p_2})}\right]\left[1-\sum_{f'}\frac{g_{ff'}}{(f'-E_{p_2})}+\frac{2g_{f_1f_2}}{(E_{p_1}-E_{p_2})}\right]\right\}\div$$

$$\div\left\{\sum_{f_1f_2}\frac{1}{(f_1-E^*_{p_1})(f_2-E^*_{p_2})}\left[\frac{1}{(f_1-E_{p_1})(f_2-E_{p_2})}+\frac{1}{(f_1-E_{p_2})(f_2-E_{p_1})}\right]\right\} \qquad (20)$$

With $E = E_{p_1}+E_{p_2}+\Delta$, and f_i means ε_{f_i}.

After eliminating χ_1 and χ_2 and observe that the 2º term in (18) is almost zero if the 2º term in (20) is zero (this correspond to eliminate the sum over i in eq. (13) and get eq. (14)), we have:

1)

$$\sum_{f_1f_2}\frac{1}{(f_1-E_{p_2})}\left(\frac{1}{(f_2-E^*_{p_1})^2(f_1-E^*_{p_2})}+\frac{1}{(f_1-E^*_{p_1})^2(f_2-E^*_{p_2})}\right)\left(1-\sum_{f'}\frac{g_{ff'}}{(f'-E_{p_1})}-\frac{2g_{f_1f_2}}{(E_{p_1}-E_{p_2})}\right)=0 \qquad (18')$$

2)

$$\sum_{f_1 f_2} \frac{1}{(f_1 - E_{p_1})} \left(\frac{1}{(f_1 - E^*_{p_1})(f_1 - E^*_{p_2})^2} + \frac{1}{(f_2 - E^*_{p_1})(f_1 - E^*_{p_2})^2} \right) \left(1 - \sum_{f'} \frac{g_{f_1 f'}}{(f' - E_{p_2})} + \frac{2 g_{f_1 f_2}}{(E_{p_1} - E_{p_2})} \right) = 0 \tag{19'}$$

We observe that we have the same exact solution[1] if we put $g_{ff'}=g$.

Some naive calculations for one and two pairs systems

For N=1 it is easy to calculate E_p by eq.(15), taking in account the term χ_1. The results is listed in table I, where we use two single-particles levels, $\varepsilon_{j_1}=0.$, $\varepsilon_{j_2}=1.$, pairs degeneracy of levels: $\Omega_{j_1}=2$, $\Omega_{j_2}=3$ and the various matrix elements are denoted by $g_{jj'}$. We list in table I, the exact diagonalization in the correspondent space (seniority zero states) and the exact result using constant matrix element[1], $g=0.5$.

For N=2, we solve (18') and (19') in two levels using single particles levels $\varepsilon_{j_1}=0.$, $\varepsilon_{j_2}=1.$, pairs degeneracy $\Omega_{j_1}=2$, $\Omega_{j_2}=2$. We have exact diagonalization and g constant calculation too (g=1). In both calculations N=1, N=2, don't take too serious the results when the g_{ij} are far from the the values 0.5 and 1.0 respectively, and note that the absolute value of Δ decrease until zero, since we have the matrix elements $g_{jj'}$ becoming $g_{ij}=g$. The total energy is obtained by summing $(E_{p_1}+E_{p_2})$ with Δ.

The author is indebted to E.V. Passos for useful discussions.

			(1)	(2)	(1')	(2')
$g_{j_1j_1}$	$g_{j_1j_2}$	$g_{j_2j_2}$	$-E_1$	$-E_1$	E_2	E_2
0.1	0.5	0.9	1.7000	1.7000	0.8000	0.8000
0.2	0.5	0.8	1.6247	1.6247	0.8247	0.8247
0.3	0.5	0.7	1.6000	1.6000	0.9000	0.9000
0.4	0.5	0.6	1.6229	1.6229	1.0229	1.0229
0.5	0.5	0.5	1.6861	1.6861	1.1861	1.1861
0.6	0.5	0.4	1.7811	1.7811	1.3811	1.3811
0.7	0.5	0.3	1.1000	1.9000	1.6000	1.6000
0.8	0.5	0.2	1.0000	2.0365	1.8365	1.8365
0.9	0.5	0.1	0.9000	2.1860	2.0860	2.0860

TABLE I (N=1)

Columns (1) and (1') refers to ground and excitate energy using eq. (15) and (2),(2') have the same meaning by exact diagonalization calculation. For g=0.5, the exact energy are respectively -1.6861 and 1.1861 by eq. (16') of ref.(1).

$g_{j_1j_1}$	$g_{j_1j_2}$	$g_{j_1j_2}$	$E_1^{(1)}+E_2^{(1)}$ (A)	Δ	Exact	$E_1^{(2)}+E_2^{(2)}$	Δ (B)	Exact	$E_1^{(3)}+E_2^{(3)}$	Δ (C)	Exact
0.6	1.0	1.4	-3.82	-.07	-4.1211	—	—	-.2899	2.43	-.08	2.4109
0.8	1.0	1.2	-4.10	-.03	-4.2165	-0.34	-.20	-.4546	2.72	-.05	2.6711
0.9	1.0	1.1	-4.22	-.01	-4.2748	-0.48	-.11	-.5388	2.84	-.03	2.8135
1.0	1.0	1.0	-4.3402	0.0000	-4.3402	-0.6222	0.0000	-.6222	2.9624	0.0000	2.9624
1.2	1.0	0.8	-4.56	0.02	-4.4922	-0.91	0.29	-.7830	—	—	3.2752
1.4	1.0	0.6	-4.75	0.04	-4.6720	-1.17	0.59	-.9314	—	—	3.6034
1.6	1.0	0.4	-4.94	0.06	-4.8784	—	—	-1.0647	—	—	3.9431

TABLE II (N=2)

Columns (A) (B) (C) are respectively the ground state and excitate states, each of them containing our calculations ($E=E_1+E_2+\Delta$) and exact diagonalization. The trace (-) means that we didn't get the root. The exact g=constant=1.0, calculation by ref.(1) gives respectively -4.3402, -0.6222, and 2.9624.

REFERENCES

(1) R.W.Richardson, N.Sherman; Nucl.Phys. 52, 221 (1964).

(2) A.Messiah; Quantum Mechanics (North-Holland Publ.Co. - Amsterdam) vol.2, pp.763.