High Energy Physics and Nuclear Physics

Volume 17, Number 3

Study of Multiplicity of Hartree-Fock Solution

Jing Xiaogong, Zhao Guoquan, Yao Yujie, Yang Shande and Wu Shishu

(Center of Theoretical Physics, Department of Physics, Jilin University, Changchun, Jilin, China)

By means of a generalized three-level solvable model, the self-consistent procedure for solving the Hartree-Fock (HF) equation is studied in detail. It is pointed that some attention should be paid to the multiplicity of the solution. Different criteria for choosing a proper solution are considered and discussed. The reason for the sudden jump of the HF solution in some force-parameter (FP) regions, the stability of the HF solution and the FP dependence of the solution are also investigated.

1. INTRODUCTION

It is well known that the approximate solutions of the nuclear many-body problem are closely related to the choice of the single particle potential. This potential is simple in form and convenient in calculation, so that it has intensively been used as an initial approximation in theoretical microscopic calculations. Since the generalized three-level solvable model can exactly be solved, it can provide us a reliable criterion to determine whether a theoretical method is good or bad. In this article, by means of the generalized three-level solvable model, we study the self-consistent procedure for solving the HF equation in detail. The calculated result shows that some attention should be paid to the multiplicity of the solution, while the criterion of the stability of the solution also cannot be ignored. Moreover, the reason of the sudden jump of the HF solution in some FP regions, the stability of the HF solution and the FP dependence of the solution are also investigated. It is expected that these conclusions will benefit the theoretical calculation of the many-body problem with the real nuclear force.

Supported by the National Natural Science Foundation of China and the Foundation of State Education Commission. Received on March 24, 1992.

2. HF EIGENVALUE EQUATION OF THREE-LEVEL SOLVABLE MODEL

The HF single particle eigenvalue equation reads

$$(t + u^{\mathrm{HF}})|\alpha\rangle = \varepsilon_\alpha^{\mathrm{HF}}|\alpha\rangle, \tag{1}$$

where the HF single particle potential u^{HF} derived from the variational principle satisfies

$$u_{\alpha\beta}^{\mathrm{HF}} = \sum_\gamma v_{\alpha\gamma\beta\gamma} n_\gamma, \tag{2}$$

where n_γ is the number of particles in the single particle state γ, and v is the two-body interaction. In the generalized three-level solvable model, since the two-body interaction exists only between the states with the same degenerate index and the Hamiltonian is independent of the degenerate index, the degenerate index of the HF single particle level is exactly the same as that of the model single particle basis $|pa\rangle$ (a is the level index, whose values can be taken as z, y and x, p is the degenerate index which can be chosen as 1, 2, 3, $\cdots$, Ω, and Ω is the degenerate degree of the single particle level), and the HF eigenvector $|p\alpha\rangle$ can be expanded as

$$|p\alpha\rangle = \sum_a |pa\rangle C_{a\alpha}. \tag{3}$$

Then one can write the HF eigenvalue equation as

$$\sum_{b=z,y,x} [u_{papb}^{\mathrm{HF}} + (\varepsilon_a - \varepsilon_\alpha^{\mathrm{HF}})\delta_{ab}] C_{b\alpha} = 0, \tag{4}$$

where ε_α is the single particle energy of the model basis, $\varepsilon_\alpha^{\mathrm{HF}}$ and $C_{b\alpha}$ ($\alpha = 1,2,3$) are the HF single particle energy and corresponding eigenvector, respectively. To simplify the problem, we only consider the full shell case, namely, $n_1 = 1$, $n_2 = n_3 = 0$.

By using

$$u_{papb}^{\mathrm{HF}} = \sum_{qcd} C_{c1}^* v_{paqcpbqd} C_{d1} \tag{5}$$

and the expression of the two-body interaction matrix element $v_{paqcpbqd}$ given in [1], a specific formula for calculating u_{papb}^{HF} can be obtained (see Appendix). It can clearly be seen that u^{HF} depends on not only the strength parameters of force (U, V, X, W, T) and the degenerate degree (Ω), but also the HF wave function C_{a1} to be calculated. In short, the equation satisfied by the HF single particle potential is no longer the eigenvalue equation in common sense, it cannot be solved by using the ordinary procedure except the self-consistent way.

In the self-consistent procedure, an initial value $C_{a1}^{(0)}$ for $C_{a1}^{(0)}$ should be given first, then u_{papb}^{HF} can be calculated, the HF eigenvalue equation can be solved, and the obtained wave function $C_{a1}^{(1)}$ and the initial value $C_{a1}^{(0)}$ can be compared. If the overlap

$$D = |\sum_a C_{a1}^{(0)} C_{a1}^{(1)}|$$

is satisfied by the required accuracy, namely, $D \geq \Delta$ (in this work $\Delta = 0.999999$), the result is self-consistent, otherwise, the previous steps should be repeated by taking $C_{a1}^{(1)}$ as the new initial value until the required accuracy is reached.

Table 1

X	$E_0(4)$	ε_1^{HF}	$\overline{H}(4)$	$B_0(4)$	ε_{min}
−0.50	−19.86	−7.58	−12.70	0.36	−1.86
		−7.55	−12.66	0.41	−2.37
		−7.46	−12.27	0.47	−4.31
−0.35	−18.35	−8.05	−13.67	0.41	0.86
		−8.01	−13.56	0.45	0.48
		−7.86	−12.92	0.50	−1.11
−0.20	−17.33	−8.54	−14.66	0.50	3.44
		−8.49	−14.51	0.51	3.18
		−8.29	−13.65	0.50	1.97

$U=0.22, V=-0.70, W=1.0, T=2.0$

Table 2

T	$E_0(4)$	ε_1^{HF}	$\overline{H}(4)$	$B_0(4)$	ε_{min}
1.40	−25.83	−11.70	−20.88	0.90	8.21
1.85	−24.24	−9.91	−17.47	0.84	3.95
		−7.83	−11.76	0.24	3.82
1.90	−24.10	−9.71	−17.10	0.83	3.41
		−8.82	−15.47	0.58	4.83
		−7.92	−11.94	0.24	3.89
1.97	−23.92	−9.43	−16.59	0.82	2.59
		−9.13	−16.43	0.63	2.35
		−8.91	−15.62	0.54	2.58
		−8.04	−12.19	0.24	3.98
1.98	−23.90	−9.39	−16.52	0.82	2.37
		−9.14	−16.45	0.63	2.55
		−8.92	−15.64	0.54	2.76
		−8.06	−12.23	0.24	4.00
1.99	−23.87	−9.35	−16.44	0.82	2.34
		−9.15	−16.47	0.63	2.74
		−8.94	−15.67	0.54	2.93
		−8.08	−12.27	0.24	4.01

$U=-0.55, V=-1.80, X=-0.40, W=-0.45$

3. CALCULATED RESULTS AND DISCUSSION

3.1 Multiplicity of Solution in HF Self-Consistent Procedure

The matrix elements of u^{HF} depend on the initial value $C_{al}^{(0)}$ of the HF wave function. There is no any restriction on $C_{al}^{(0)}$ besides the normalization condition

$$\sum_a |C_{al}^{(0)}|^2 = 1.$$

Therefore, in principle, one has many different choices for the initial value, and consequently many sets of self-consistent solutions for one specific set of FP. This is the multiplicity of the solution in the HF self-consistent procedure. We use 96 different normalized initial values in the calculation. For example, as $\Omega = 4$, $\varepsilon_x = 2.5$, $\varepsilon_y = 2.0$ and $\varepsilon_z = 0.0$ (the same values here after), the calculated results with different FP are given in Tables 1 and 2.

In these tables,

$$\bar{H}(4) = \langle \Phi_0(4) | \hat{H} | \Phi_0(4) \rangle,$$
$$B_0(4) = |\langle \Psi_0(4) | \Phi_0(4) \rangle|,$$

where $E_0(4)$ and $|\Psi_0(4)\rangle$ are the exact ground state energy and eigenvector for the $N = 4$ particle system, respectively, and $|\Phi_0(4)\rangle$ is the Slater determinant constructed by the HF wave functions C_{al} in the same system.

In Table 1, there are three sets of different self-consistent solutions for each set of parameters. In Table 2, the number of solutions increases from 1 to 4 with the increasing parameter T. The direct reason which causes multiple solutions is that u^{HF} depends on the HF wave function C_{al} to be solved, and its origin is that the variational principle would possibly give many extreme values of $\bar{H}(4)$.

In order to choose a required stable solution from obtained solutions, one should judge the stabilities of solutions first. Thouless [2] proposed the condition of a stable HF solution. If $\mathscr{E}$ satisfies the matrix equation

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = \mathscr{E} \begin{pmatrix} X \\ Y \end{pmatrix} \tag{6}$$

and its minimal value $\mathscr{E}_{min}$ satisfies $\mathscr{E}_{min} > 0$, the HF solution is stable. Then,

$$A_{minj} = (\varepsilon_m - \varepsilon_i)\delta_{mn}\delta_{ij} + V_{mjin},$$
$$B_{minj} = V_{mnij}, \tag{7}$$

where m and n are single particle states, while i and j are single hole states. $\mathscr{E}_{min}$ values obtained above are given in Tables 1 and 2. It is obvious that in Table 1, all HF solutions are not stable when $X = -0.50$, the first two sets of solution are stable when $X = -0.35$ and all solutions are stable when $X = -0.20$. Also, all solutions are stable in Table 2. A detailed discussion on the unstable solution will be given elsewhere.

The second step is to select the solutions which satisfy certain requirements from stable solutions for some specific problems. Since the HF single particle potential is derived by using the variational principle, one commonly determines the HF solution by taking the minimal value of $\bar{H}(4)$ (called

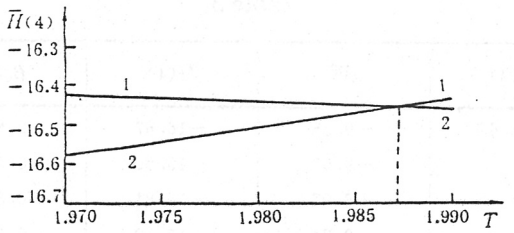

Fig. 1

model 1). Thus, one should choose the first sets of solution in the cases of $X = -0.35$ and $X = -0.20$, respectively in Table 1, while in Table 2, the first sets of solution in the cases of $T = 1.4$-1.98, respectively, and the second set of solution in the case of $T = 1.99$. It is clear that the solutions chosen in this way can ensure the optimized results in the $\bar{H}(4)$ calculation. However, the method mentioned above is not an unique choice. For instance, one may start with the maximum overlap principle of wavefunction, or may choose the solution according to the maximum value of $B_0(4)$ (called model 2). By neglecting higher order terms, namely, considering the HF solution as a good approximation, models 1 and 2 give fully coincident results in the $T = 1.40$-1.98 region. But, in some cases, they do offer different results. For example, in Table 1, when $X = -0.35$ and $X = -0.20$ one should choose the first sets of solution, respectively, in model 1 and the second sets of solution, respectively, in model 2, and in Table 2, when $T = 1.99$ one has to take the second and first sets of solution in models 1 and 2, respectively. Here, the inconsistency in two tables provides a possibility to choose a proper HF solution for a specific problem. If the results of $\bar{H}(4)$ are concerned, model 1 should be chosen. But if the results of $B_0(4)$ are more important, model 2 must be adopted. Moreover, we should pointed out that there may exist other models besides models 1 and 2.

3.2 Sudden Jump of HF Solution Which Incorporates Phase Change of System

We pointed out in [1] that the HF solution had the sudden jump in the certain FP region, and discussed the relation between the sudden jump and the phase change of the system in [2]. In this article, we investigate the reason which causes such sudden jump when the exact solution of the system does not have any phase change in the same FP region. For example, in Table 2, the HF solution has a sudden jump in model 1 when T varies from 1.98 to 1.99, while the system does not have phase change. In order to explain the reason for such sudden jump we plot the curves of $\bar{H}(4)$ with respect to the parameter T for two lowest stable solutions, respectively, in Fig. 1. From Fig. 1 one sees that both curves vary smoothly with respect to T. They cross each other at $T = 1.987$. According to model 1, one should choose the first set of solution when $T < 1.987$, and the second set of solution when $T > 1.987$. In fact, the difference between these two sets is evident, so that the sudden jump takes place around $T = 1.987$. The direct reason of the sudden jump is that the quantity for choosing solution has an intersection point.

In order to find the second reason for the sudden jump, we list related results in Table 3. In this table the other FP values are the same as those in Table 2. The $\mathscr{E}_{\min}$ values in Table 3 tell us that all solutions are stable. When the difference of H(4) between two solutions is small but the difference of $B_0(4)$ is larger, one may also use the model 2 to choose the solution. Therefore, one should take the third set of solution when $T \leq 2.09$ and the first set of solution when $T = 2.10$. The apparent difference between two solutions results the sudden jump of the HF solution. The direct reason of such sudden jump is that the third set of solution has less stability with increasing T, and disappears at $T = 2.10$.

Table 3

T	$E_0(4)$	ε_i^{HF}	$H(4)$	$B_0(4)$	$\mathscr{E}_{min}$
2.08	−23.67	−9.28	−16.67	0.618	4.13
		−9.07	−15.90	0.532	4.21
		−8.97	−15.81	0.803	0.75
		−8.24	−12.59	0.245	4.13
2.09	−23.65	−9.29	−16.70	0.617	4.27
		−9.08	−15.93	0.532	4.34
		−8.92	−15.75	0.801	0.29
		−8.25	−12.63	0.245	4.14
2.10	−23.63	−9.30	−16.72	0.617	4.40
		−9.10	−15.96	0.531	4.46
		−8.27	−12.66	0.245	4.15

Table 4

Parameter value	$\mathscr{E}_{min}(T)$	$\mathscr{E}_{min}(W)$	$\mathscr{E}_{min}(X)$	$\mathscr{E}_{min}(V)$	$\mathscr{E}_{min}(U)$
0.2	1.60	1.60	1.02	0.80	1.85
0.4	1.02	1.20	−0.16	−0.40	1.75
0.6	0.43	0.80	−1.36	−1.60	
0.8	−0.16	0.40	−2.56	−2.80	
1.0	−0.76		−3.76	−4.00	

In one word, the calculated result shows that the sudden jump of the HF solution in the FP region mentioned above is independent of the choice of model, but the position of the sudden jump depends. Since the system does not have the phase change in this region, the sudden jump of the HF solution is caused by the adoption of the HF approximate method itself and does not necessarily related to the real phase change of the system.

3.3 Relation Between Stability of HF Solution and FP

In order to understand the relation between the stability of the HF solution and the two-body interaction, we systematically study each strength parameter of force by setting other strength parameters of force to be zero, and list calculated results in Table 4. The result indicates that with the increase of the strength parameter of force, i.e. with the enhancement of the two-body interaction the HF solution becomes less stable, unstable, until disappearance.

APPENDIX

$$
\begin{aligned}
u^{\mathrm{HF}}_{pzpz} &= C^{*}_{z1}[U(\Omega-1)(C_{y1}+C_{x1})] \\
&\quad + C^{*}_{y1}[U(\Omega-1)C_{z1}-2WC_{y1}+(U\Omega-T)C_{x1}] \\
&\quad + C^{*}_{x1}[U(\Omega-1)C_{z1}+(U\Omega-T)C_{y1}-2WC_{x1}];
\end{aligned}
$$

$$
\begin{aligned}
u^{\mathrm{HF}}_{pzpy} &= C^{*}_{z1}[U(\Omega-1)C_{z1}+2V(\Omega-1)C_{y1}+2X(\Omega-1)C_{x1}] \\
&\quad + C^{*}_{y1}[2W\Omega C_{z1}+U(\Omega-1)C_{y1}+(\Omega T-U)C_{x1}] \\
&\quad + C^{*}_{x1}[(\Omega T-U)C_{z1}+2X(\Omega-1)C_{y1}+(\Omega U-T)C_{x1}]; \\
u^{\mathrm{HF}}_{pzpx} &= C^{*}_{z1}[U(\Omega-1)C_{z1}+2X(\Omega-1)C_{y1}+2V(\Omega-1)C_{x1}] \\
&\quad + C^{*}_{y1}[(T\Omega-U)C_{z1}+(U\Omega-T)C_{y1}+2X(\Omega-1)C_{x1}] \\
&\quad + C^{*}_{x1}[2W\Omega C_{z1}+(\Omega T-U)C_{y1}+U(\Omega-1)C_{x1}]; \\
u^{\mathrm{HF}}_{pypy} &= C^{*}_{z1}[-2WC_{z1}+U(\Omega-1)C_{y1}+(U\Omega-T)C_{x1}] \\
&\quad + C^{*}_{y1}[U(\Omega-1)(C_{z1}+C_{x1})] \\
&\quad + C^{*}_{x1}[(U\Omega-T)C_{z1}+U(\Omega-1)C_{y1}+2WC_{x1}]; \\
u^{\mathrm{HF}}_{pypx} &= C^{*}_{z1}[(U\Omega-T)C_{z1}+(T\Omega-U)C_{y1}+2X(\Omega-1)C_{x1}] \\
&\quad + C^{*}_{y1}[2X(\Omega-1)C_{z1}+U(\Omega-1)C_{y1}+2U(\Omega-1)C_{x1}] \\
&\quad + C^{*}_{x1}[(T\Omega-U)C_{z1}+2W\Omega C_{y1}+U(\Omega-1)C_{x1}]; \\
u^{\mathrm{HF}}_{pxpx} &= C^{*}_{z1}[-2WC_{z1}+(U\Omega-T)C_{y1}+U(\Omega-1)C_{x1}] \\
&\quad + C^{*}_{y1}[(U\Omega-T)C_{z1}-2WC_{y1}+U(\Omega-1)C_{x1}] \\
&\quad + C^{*}_{x1}[U(\Omega-1)(C_{z1}+C_{y1})].
\end{aligned}
$$

and

$$
u^{\mathrm{HF}}_{pypz}=u^{\mathrm{HF}}_{pzpy}; \qquad u^{\mathrm{HF}}_{pxpz}=u^{\mathrm{HF}}_{pzpx}; \qquad u^{\mathrm{HF}}_{pxpy}=u^{\mathrm{HF}}_{pypx}.
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