Comparison of two kinds of truncations

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(Received 3 October 1988)

Two kinds of truncations in the microscopic calculation of nuclear low-lying excited states, the many-particle configuration truncation and the single-particle level truncation, are compared. The distinction between them and the advantage of the former over the latter are discussed.

I. INTRODUCTION

In medium and heavy deformed nuclei, the single-particle levels near the Fermi surface are, roughly speaking, uniformly distributed. The average spacing between adjacent levels is approximately[1]

$$d \sim 50A^{-1}\ \mathrm{MeV}\ . \tag{1}$$

In any practical microscopic calculation for a deformed nucleus certain truncations must be made. Usually, in various microscopic calculations (e.g., shell-model calculations,[2,3] Bardeen-Cooper-Schrieffer (BCS),[4] Hartree-Fock-Bogoluibov,[5] etc.), a single-particle level (SPL) truncation is adopted. In the framework of this kind of truncation all the single-particle levels, ϵ_ν, lying in the region

$$|\epsilon_\nu - \epsilon_F| < \epsilon_c \quad (\epsilon_F,\ \text{Fermi energy}) \tag{2}$$

are involved in the calculation. This means that all the levels $\epsilon_\nu < \epsilon_F - \epsilon_c$ are occupied and all the levels $\epsilon_\nu > \epsilon_F + \epsilon_c$ are vacant. Alternatively, in the particle-number-conserving (PNC) treatment for nuclear pairing correlation,[6,7] a new kind of truncation, the many-particle configuration (MPC) truncation, is suggested. In this approach all the many-particle configurations of energy E

$$(E - E_0) < E_c \tag{3}$$

are taken into account in the diagonalization of the Hamiltonian, where E_0 is the energy of the lowest (ground) configuration. Obviously , these two kinds of truncations coincide with each other as both ϵ_c and E_c tend to infinity. But for finite energy truncation there are some important distinctions between them which have not attracted general attention yet.[8] In this paper the advantage of the MPC truncation over the SPL truncation is discussed in some detail. It will be shown that in the usual SPL truncation, on the one hand, a great number of configurations, which are very unimportant for the low-lying excited states of a many-particle system, are involved and make the computation very tedious and time consuming, and on the other hand, a large number of relatively important configurations are omitted, hence some results thus obtained are unsatisfactory from the physical point of view. Also it will be shown that the defects encountered in the SPL truncation do not occur in the MPC truncation and a rather accurate solution to the low-lying excited states can be obtained much more easily than that in the SPL truncation. The eigenvalue problem of the pairing Hamiltonian is taken as an illustrative example. Similar discussion can be extended to the eigenvalue problem of the cranked shell-model (CSM) Hamiltonian[9,10] and pairing plus quadrupole-quadrupole interaction.[11]

As usual, the pairing Hamiltonian is expressed as follows:

$$H = \sum_\nu \epsilon_\nu a_\nu^\dagger a_\nu - G \sum_{\mu,\nu>0} a_\mu^\dagger a_{\bar\mu}^\dagger a_{\bar\nu} a_\nu \ , \tag{4}$$

where ϵ_ν is the single-particle energy (twofold degenerate), ν denotes the single-particle state and $\bar\nu$ its time-reversal state, and G is the average strength of pairing interaction. For convenience, we assume a uniformly distributed single-particle level scheme which may be considered as a prototype of deformed nuclei.[3] The spacing between the adjacent levels is taken as the energy unit, $d=1$; see Fig. 1. However, the conclusions drawn in the following remain valid for a nonuniformly distributed single-particle level scheme.

II. SPL TRUNCATION

A usual shell-model calculation using the SPL truncation with $2\epsilon_c = 10$ was carried out. In this case, ten single-particle levels around the Fermi surface and ten particles are involved and the dimension of the configuration space of seniority $v=0$ (i.e., fully paired configurations) is $D(2\epsilon_c=10)=252$. For $G=0.5$ the pairing Hamiltonian (4) is diagonalized exactly in this configuration space and the calculated low-lying excited spectra of this system are 0, 2.806, 4.716, 4.716, 6.662, 6.662, 7.149, ...

Now let us investigate the properties of the ground and the first excited states.

(a) The lowest configuration is expressed as $|\underline{54321}\rangle$, which means that all the single-particle levels below ϵ_F (i.e., $\underline{1}$, $\underline{2}$, $\underline{3}$, $\underline{4}$, and $\underline{5}$) are occupied. The highest configuration is $|12345\rangle$, i.e., all the five pairs of particles are excited to the levels above ϵ_F and the corresponding configuration energy is $(E-E_0)=50$. Calculation shows that for the low-lying excited states the number of important configurations is very limited. The main

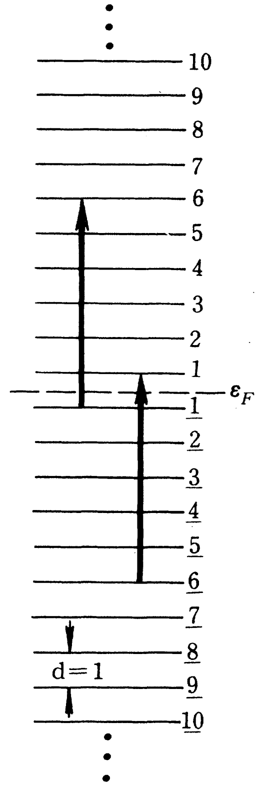

FIG. 1. Single-particle level scheme. ϵ_F denotes the Fermi energy. The spacing between the adjacent levels is taken as the energy unit, $d=1$. For clarity, the single-particle levels below ϵ_F are labeled by underlined numbers.

configurations with weight larger than 1% are listed in Table I. It is found that the energies of all these main configurations are smaller than 10. Calculations with larger ϵ_c show that all the configurations with weight $>1\%$ have been involved in the SPL truncation $2\epsilon_c=10$. The weight of the lower-lying configurations $E-E_0\leq 10$ exceeds 94%. The weights of the configurations within various energy regions are listed in Table II. Obviously, while the number of the higher configurations increases with increasing $(E-E_0)$, the corresponding weights in the low-lying excited states decrease steeply. For example, the weight of the configurations with $E-E_0>20$ only amounts to 0.436%.

(b) In the SPL truncation, while the overwhelming majority of the configurations considered are very unimportant for the low-lying excited states, many relatively important configurations are omitted. In the SPL truncation $|\epsilon_\nu-\epsilon_F|<\epsilon_c$, the highest configuration energy is $2\epsilon_c^2/d$. However, numerous configurations of energy $(E-E_0)>2\epsilon_c$ are omitted. For example, when a pair of particles is excited to ϵ_ν $(\nu>5$, e.g., configuration $|\underline{5}\underline{4}\underline{3}\underline{2}6\rangle)$, or an empty level below ϵ_ν $(\nu<\underline{5})$ is created (see the arrows shown in Fig. 1), the corresponding configurations are relatively important, but they are omitted in the SPL truncation with $2\epsilon_c=10$. A more detailed discussion will be given in Sec. III. If we wish to include these configurations in the SPL truncation, we have to increase ϵ_c. However, the dimension of configuration space is

$$D(\epsilon_c)=\frac{(2\epsilon_c/d)!}{(\epsilon_c/d)!(\epsilon_c/d)!} \tag{5}$$

which increases drastically with increasing ϵ_c (e.g., $D=184756$ for $2\epsilon_c=20$), hence a vast number of unimportant configurations will be involved and the computation becomes really tremendous, either by numerical diagonalization or by the Richardson method.[2,3]

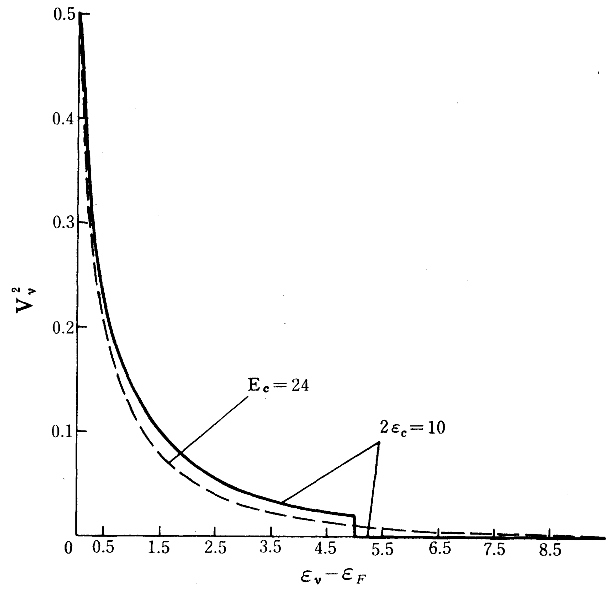

FIG. 2. The occupation probability of individual single-particle levels above the Fermi surface by a pair of particles. For the single-particle levels below ϵ_F, $V_{\underline{\nu}}^2=-1-V_\nu^2$. The solid line is the result obtained by using the SPL truncation with $2\epsilon_c=10$ and $G=0.5$. The dashed line represents that by the MPC truncation with $E_c=24$ and $G=0.3936$. The renormalization of the pairing strength G has been taken into account in the MPC truncation to reproduce the same first excited level as that in the SPL truncation with $2\epsilon_c=10$.

(c) It is worthwhile to investigate the occupation probability of individual single-particle levels by a pair of particles. The results for $2\epsilon_c=10$ is displayed in Fig. 2. It can be seen that jumps occur around $|\epsilon-\epsilon_F|=5$, which seems unsatisfactory from the assumption of uniformity of the single-particle level distribution. To weaken such a defect we have to increase ϵ_c. Also it will lead to a terrible amount of computation.

III. MPC TRUNCATION

In the PNC treatment for the pairing Hamiltonian[6,7] the many-particle configuration truncation is adopted instead of the usual SPL truncation. Calculation shows that the MPC truncation is not only more reasonable from the theoretical point of view, but also more effective for treating the low-lying excited states of a many-

TABLE I. The main configurations and their weights in two lowest states calculated by using the SPL truncation with $2\epsilon_c = 10$.

Configurations	$\vert\underline{54321}\rangle$	$\vert\underline{5432}1\rangle$	$\vert\underline{5432}2\rangle$	$\vert\underline{5431}1\rangle$	$\vert\underline{5432}3\rangle$	$\vert\underline{5431}2\rangle$	$\vert\underline{5421}1\rangle$	$\vert\underline{5432}4\rangle$	$\vert\underline{543}12\rangle$	$\vert\underline{5421}1\rangle$	Total weight
Ground state	0.6013	0.1138	0.0411	0.0411	0.0201	0.0175	0.0201	0.0117	(0.0051)	0.0117	88.4%
1st excited state	0.2780	0.5526	0.0283	0.0283	(0.0079)	(0.0000)	(0.0079)	(0.0034)	0.0173	(0.0034)	92.7%

TABLE II. The weights of configurations within various energy regions in the SPL truncation with $2\epsilon_c = 10$.

Configuration energy $(E-E_0)$	[0,10]	(10,12]	(12,14]	(14,16]	(16,18]	(18,20]	(20,30]	(30,50]
Number of configurations	19	9	11	14	16	18	96	69
Ground state	0.940 06	0.022 40	0.014 62	0.009 56	0.005 79	0.003 20	0.004 20	0.000 16
1st excited state	0.948 52	0.017 43	0.015 30	0.008 60	0.004 89	0.002 37	0.002 78	0.000 12

TABLE III. The configurations involved in the MPC truncation with $E_c = 16$. In the notation such as $|\ldots\underline{54321}\rangle$ the ellipsis $(\ldots)$ means all the single-particle levels below the lowest level indicated explicitly (i.e., $\underline{5}$) are occupied.

$E-E_0$	Configurations							
0	$\vert\ldots\underline{54321}\rangle$							
2	$\vert\ldots\underline{5432}1\rangle$							
4	$\vert\ldots\underline{5432}2\rangle$	$\vert\ldots\underline{5431}1\rangle$						
6	$\vert\ldots\underline{5432}3\rangle$	$\vert\ldots\underline{5431}2\rangle$	$\vert\ldots\underline{5421}1\rangle$					
8	$\vert\ldots\underline{5432}4\rangle$	$\vert\ldots\underline{5431}3\rangle$	$\vert\ldots\underline{543}12\rangle$	$\vert\ldots\underline{5421}2\rangle$	$\vert\ldots\underline{5321}1\rangle$			
10	$\vert\ldots\underline{5432}5\rangle$	$\vert\ldots\underline{5431}4\rangle$	$\vert\ldots\underline{543}13\rangle$	$\vert\ldots\underline{5421}3\rangle$	$\vert\ldots\underline{542}12\rangle$	$\vert\ldots\underline{5321}2\rangle$	$\vert\ldots\underline{64321}1\rangle$	
12	$\vert\ldots\underline{5432}6\rangle$*	$\vert\ldots\underline{5431}5\rangle$	$\vert\ldots\underline{543}14\rangle$	$\vert\ldots\underline{543}23\rangle$	$\vert\ldots\underline{5421}4\rangle$	$\vert\ldots\underline{542}13\rangle$	$\vert\ldots\underline{541}12\rangle$	$\vert\ldots\underline{5321}3\rangle$
	$\vert\ldots\underline{532}12\rangle$	$\vert\ldots\underline{64321}2\rangle$	$\vert\ldots\underline{754321}1\rangle$*					
14	$\vert\ldots\underline{5432}7\rangle$*	$\vert\ldots\underline{5431}6\rangle$*	$\vert\ldots\underline{543}15\rangle$	$\vert\ldots\underline{543}24\rangle$	$\vert\ldots\underline{5421}5\rangle$	$\vert\ldots\underline{542}14\rangle$	$\vert\ldots\underline{542}23\rangle$	$\vert\ldots\underline{541}13\rangle$
	$\vert\ldots\underline{5321}4\rangle$	$\vert\ldots\underline{532}13\rangle$	$\vert\ldots\underline{531}12\rangle$	$\vert\ldots\underline{64321}3\rangle$	$\vert\ldots\underline{6432}12\rangle$	$\vert\ldots\underline{754321}2\rangle$*	$\vert\ldots\underline{8654321}1\rangle$*	
16	$\vert\ldots\underline{5432}8\rangle$*	$\vert\ldots\underline{5431}7\rangle$*	$\vert\ldots\underline{543}16\rangle$*	$\vert\ldots\underline{543}25\rangle$	$\vert\ldots\underline{543}34\rangle$	$\vert\ldots\underline{5421}6\rangle$*	$\vert\ldots\underline{542}15\rangle$	$\vert\ldots\underline{542}24\rangle$
	$\vert\ldots\underline{541}14\rangle$	$\vert\ldots\underline{541}23\rangle$	$\vert\ldots\underline{5321}5\rangle$	$\vert\ldots\underline{532}14\rangle$	$\vert\ldots\underline{532}23\rangle$	$\vert\ldots\underline{531}13\rangle$	$\vert\ldots\underline{521}12\rangle$	$\vert\ldots\underline{64321}4\rangle$
	$\vert\ldots\underline{6432}13\rangle$	$\vert\ldots\underline{6431}12\rangle$	$\vert\ldots\underline{754321}3\rangle$*	$\vert\ldots\underline{75432}12\rangle$*	$\vert\ldots\underline{8654321}2\rangle$*	$\vert\ldots\underline{97654321}1\rangle$*		

TABLE IV. The dimension of configuration space in the MPC truncation.

Truncated configuration energies E_c	10	12	14	16	18	20	22	24
Dimensions of configuration space $D(E_c)$	19	30	45	67	97	139	195	272
Numbers of configurations omitted in the SPL truncation $2\epsilon_c = 10$	0	2	6	14	28	52	89	146

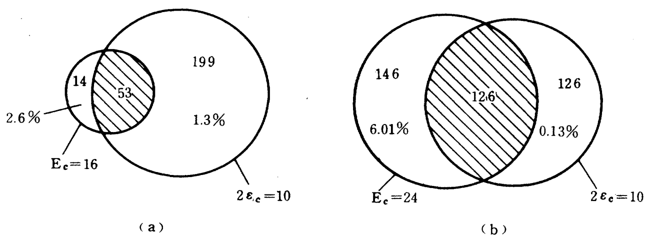

FIG. 3. Pictorial illustration of configuration spaces in two kinds of truncations. The configuration spaces are sketched by circles. The overlap between circles denotes the common part of two spaces. The numbers of configurations in each part as well as the corresponding weights in the ground state are also shown.

particle system. The defects of the SPL truncation mentioned above disappear in the MPC truncation. Accurate solutions to the low-lying excited states can be obtained more easily by using the MPC truncation. As an illustrative example the configurations considered in the MPC truncation $E_c = 16$ are listed in Table III. In this case 16 single-particle levels around the Fermi surface (i.e., $\underline{8}$, $\underline{7}$, $\underline{6}$, $\underline{5}$, $\underline{4}$, $\underline{3}$, $\underline{2}$, $\underline{1}$, 1, 2, 3, 4, 5, 6, 7, and 8) and 16 particles are involved in the calculation. The dimension of the configuration space is $D(E_c=16)=67$. Among these 67 configurations 14 configurations (denoted by * in Table III) are omitted in the SPL truncation with $2\epsilon_c=10$ (see Fig. 3). Calculation shows that for the low-lying excited states these omitted configurations are relatively more important. In fact, 12 configurations among them are with weight larger than 0.1% in the ground state and the total weight of these omitted configurations is 2.6%. As mentioned above, the dimension of the configuration space in the SPL truncation $2\epsilon_c=10$ is $D(2\epsilon_c=10)=252$. It is seen that 199 of these configurations do not enter into the configuration space for $E_c=16$ because their configuration energies are larger than 16 (see Fig. 3). It is interesting to note that the total weight of such numerous configurations is only 1.3% in the ground state. A similar situation exists for the other low-lying excited states. Therefore the results obtained in the MPC truncation with $E_c=16$ $(D=67)$ are more accurate than those obtained in the SPL truncation with $2\epsilon_c=10$ $(D=252)$, though the computational work for the latter is much more time consuming than that for the former.

The dimensions of configuration space for various E_c are listed in Table IV. The numbers of configurations which were omitted in the SPL truncation with $2\epsilon_c=10$ are also listed in the third row. Calculations for various E_c show that all the main configurations (weight $\geq 1\%$) lie in the region $(E-E_0)\leq 10$. Thus for different values of E_c (>10) almost the same low-lying excited spectra and wave functions can be obtained provided a renormalization of the average pairing strength parameter G is taken into account (see Fig. 4).

In the MPC truncation with $E_c=24$, 24 single-particle levels around the Fermi surface and 24 particles are in-

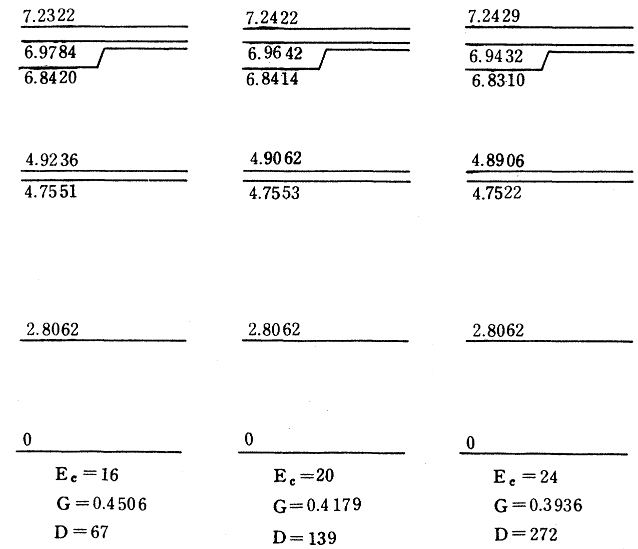

FIG. 4. The lower-lying spectra calculated with different MPC energy truncation. They are almost the same when a proper renormalization of the pairing strength G is taken into account.

volved in the calculation. The dimension of configuration space, $D(E_c=24)=272$, is close to that in the SPL truncation $2\epsilon_c=10$. Thus the computational work is comparable in both cases. However, calculations show that for the ground state while the weight of the 146 configurations (see Fig. 3) which are involved in the MPC truncation $(E_c=24)$ but omitted in the SPL truncation $(2\epsilon_c=10)$ amounts to 6.01%, the 126 configurations which are included in the SPL truncation $(2\epsilon_c=10)$ but omitted in the MPC truncation $(E_c=24)$ amount only to 0.133%. A similar conclusion holds for the other low-lying excited states. Thus the results obtained in the MPC truncation are much more accurate and reliable than those obtained in the SPL truncation.

In summary, either from the many-body character of the problem or from the practical point of view, the advantage of the MPC truncation over the SPL truncation is obvious in the microscopic calculation for well-deformed nuclei. It is not difficult to obtain a rather accurate solution to the low-lying excited states in the MPC truncation, which is adopted in the PNC method for treating the pairing Hamiltonian,[6,7] the cranked shell-model Hamiltonian,[9,10] and the pairing plus quadrupole-quadrupole interaction.[11] Moreover, it should be emphasized that the Pauli principle (including the blocking effect), which is considered as very complicated for treating the pairing interaction,[2,12] is taken into account exactly in the PNC code. The conclusions drawn above, based on the assumption of a uniformly distributed single-particle level scheme, remain quantitatively valid for rather realistic single-particle level schemes. However, if there exists a very wide gap in the vicinity of the Fermi surface in the single-particle level scheme, this advantage would be depressed.

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