Configurational quasidegeneracy and the liquid drop model

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Zamick *et al.* recently reported on a series of Hartree-Fock calculations of light nuclei with Skyrme interaction in which they observed a near degeneracy of states corresponding to different fillings of the single-particle levels. We will present here a possible explanation for these facts using very simple arguments based on the liquid drop model.

Zamick *et al.*[1-3] (see also Ref. 4) asked the following question: Let us consider different fillings of the single-particle level scheme and perform a Hartree-Fock calculation of the corresponding configurations with a Skyrme interaction, allowing deformation for such nuclei as ^{4}He, ^{16}O, and ^{40,48}Ca, which traditionally are regarded as spherical. What excitation energies correspond to such states as 1p-1h, 2p-2h, . . . , 8p-8h, etc.? The first and wrong guess would be that the excitation energy must be of the order of $n\hbar\omega$, where n is the number of particle-hole pairs excited. Obviously such a rough estimate is wrong, since one has to include the residual interaction among particles and holes, which will be different for L,S,T quantum numbers of the p-h pair, and also a relatively large rearrangement energy, when the number of p-h pairs is large. Then one has something which can be dubbed as a p-h condensate. A typical example is ^{16}O, in which the configuration 4p-4h has an unexpected low excitation energy in a self-consistent treatment, about 10 MeV.[1-4] Such a state, strictly speaking, is not a pure 4p-4h excitation of the ground state, since the nucleus is strongly deformed in this case. The corresponding occupied single-particle orbitals states are only generically associated with the particle states characteristic for the ground state, in the same way as are the single-particle levels in a Nilsson scheme for different deformations. The same kind of behavior has been put in evidence in several nuclei and for different such np-nh "excitations."[1-4] It is unlikely that the effective Skyrme interaction used in such calculations fails to describe the physics of such states and one has to take these results at face value. Nevertheless, the nagging question "Why does this happen?" remains unanswered.

It was remarked a long time ago by Hill and Wheeler[5,6] that nuclei behave in a different manner under small and large deformations. In order to find the stiffness of nuclei for small deformation, one usually applies the linear-response theory to small external fields. Under the action of small external fields, the nuclear density is slightly deformed through the excitation of 1p-1h pairs. However, the distribution of nucleons over the single-particle levels remains, loosely speaking, unchanged. This situation corresponds to what Hill and Wheeler called rapid deformations of the single-particle field, and the corresponding stiffness and excitation energies are computed in random phase approximation (RPA). The response of nuclei to small external fields amounts to a local deformation of the Fermi sphere and the corresponding type of excitations in an infinite system is the so-called zero sound.[7] For a proper estimate of the excitation energies and strengths one has to take into account the residual interaction among the 1p-1h excitations. If the amplitude of the external field becomes too large, then deforming the Fermi sphere is energetically too costly[5,8-10] and a more favorable configuration corresponds to a redistribution of the nucleons among the single-particle levels. For different single-particle configurations one obtains, a linear-response approach, what Hill and Wheeler called potential curves for rapid deformation. The curve obtained by smoothly joining the minima of these potential curves for rapid deformations will give the potential curve for slow deformations.[5] The mechanism envisaged by Bertsch[9] for switching from one single-particle configuration to another was through the pairing interaction, which takes two particles from one orbital and transfers them to another one. One can think also of transferring at once particles from different orbitals, and probably such a process has a slightly less but comparable amplitude in the absence of a pairing condensate. Bertsch[9] derived a simple formula for the required "jump" or "hopping" in deformation, needed to switch from one configuration to another:

$$n=\beta\sqrt{5/12\pi}\,A\ , \tag{1}$$

where A is the atomic number. The potential curve for slow deformations of the nucleus has been identified[5,8] with the potential energy of the liquid drop model.

Since the parameters of the liquid drop formula are known very well,[8] and from them one can also easily find the stiffness of the potential energy of a given nucleus for slow deformations, a natural approach will be to estimate the excitation energies corresponding to different deformations β and by using Bertsch's formula, Eq. (1), to determine the corresponding number of particle-hole "excitations." The same quantity can be roughly determined from a Nilsson scheme.[11] One can determine for which deformations one has a level crossing and, consequently, when a particle transfer from one orbital to another becomes "easy." For the total energies we used the liquid drop formula[8]

$$E=-c_1A+c_2A^{2/3}+c_3Z^2/A^{1/3}-c_4Z^2/A\ ,$$

$$c_{1,2}=a_{1,2}\left[1-\kappa\left[\frac{N-Z}{A}\right]^2\right]\ ,$$

$$a_1=15.677\ \text{MeV},\quad a_2=18.56\ \text{MeV}\ ,$$

$$c_3=0.717\ \text{MeV},\quad c_4=1.211\,29\ \text{MeV}\ ,$$

$$\kappa=1.79\ ,$$

where the first term is the volume contribution, the second is the surface contribution, the third is the Coulomb energy, and the fourth is a correction to the Coulomb energy due to the diffuseness of the nuclear surface. The deformation energy for quadrupole deformation is[8] ($\gamma=0$ and only quadratic terms in β)

$$E_{\text{def}}=(\tfrac{2}{5}c_2A^{2/3}-\tfrac{1}{5}c_3Z^2/A^{1/3})\frac{5}{4\pi}\beta^2\ .$$

The results for deformations and binding energies using the preceding formulas for ^{16}O and ^{40}Ca are given in Tables I and II. The overall agreement with the results of the Hartree-Fock calculations[3] is good. From the Nilsson scheme,[11] the values for β in ^{40}Ca for $n=4$ and 8 are approximately equal to 0.3 and 0.6, respectively. In the light of these numbers, the real question seems to be not why the np-nh states with large values of n are so low, but rather, why, e.g., the 2p-2h states are so high in the Hartree-Fock approximation in comparison with the liquid drop formula.

The differences between the Hartree-Fock and liquid drop model energies are of the order of the corresponding shell corrections and pairing energies in this mass region.[8] We did not take into account the odd-even effect in the liquid drop model (LDM), which has an amplitude of a few MeV in these nuclei.[8,12] One can improve the agreement between the Hartree-Fock (HF) and LDM values for the ground states by doing this; however, it is not very clear to us how to compare the corresponding numbers for finite deformations. The magnitude of these corrections depends strongly on the nuclear shape and single-particle level densities, which can be determined in a quite sophisticated numerical approach only, which must include the determination of an optimal shape for each deformation. For large deformations, the single-particle level distribution is more uniform than for small deformations, which implies that the amplitude of these microscopic corrections will diminish as one will approach the saddle point corresponding to fission. For such nuclear shapes, the classical single-particle trajectories become chaotic, due to the presence of the neck, which at the quantum level corresponds to a more or less constant single-particle level density and absence of shell effects. The shell effects will become important again when the two fragments will separate. On the other hand, the pairing can play a relatively important role near the saddle point, due to the relatively high single-particle level density (no shells), but the overall gain in total energy will amount only to a few MeV as usual. This qualitative argument agrees with the numbers obtained in Ref. 3.

TABLE I. Deformations and total energies (in MeV) in ^{16}O according to Hartree-Fock results[3] with Skyrme III interaction and liquid drop model,[8] corresponding to n excited p-h pairs. The deformation used in the liquid drop model was computed according to Eq. (1).[9] $E_{\text{LDM}}(2)$ was computed using only the quadratic term in deformation β. $E_{\text{LDM}}(6)$ was computed using terms up to sixth order in β.[13]

n	β_{HF}	β_{LDM}	E_{HF}	$E_{\text{LDM}}(2)$	$E_{\text{LDM}}(6)$
0	0	0	−128.0	−119.3	−119.3
2	0.24	0.34	−112.9	−117.2	−117.3
4	0.63	0.69	−112.5	−111.1	−112.8
6	0.73	1.03	−96.3	−100.9	−107.7
8	0.82	1.37	−85.5	−86.6	−103.3

TABLE II. The same as in Table I but for ^{40}Ca.

n	β_{HF}	β_{LDM}	E_{HF}	$E_{\text{LDM}}(2)$	$E_{\text{LDM}}(6)$
0	0	0	−341.3	−337.4	−337.4
2	0.12	0.14	−330.8	−336.8	−336.8
2	0.13		−331.8		
4	0.32	0.27	−329.2	−335.2	−335.4
6	0.44	0.41	−327.8	−332.6	−333.1
8	0.55	0.55	−329.9	−328.9	−330.3

One can see from Tables I and II that there is a better agreement among the two sets of numbers at finite deformations, which fact seems perfectly reasonable in such a case. The agreement is also better for calcium, where one can expect that the LDM is a more reasonable approximation. In estimating the LDM deformation energies we did not take into account terms beyond second order in β. Considering higher-order terms in β along with higher multipoles will only make the liquid drop even less stiff and, consequently, the LDM estimates in Tables I and II are only upper estimates for large enough deformations. The main correction term is very likely to be due to the appearance of the saddle point along the path leading to fission, and the energy deformation curve will be bent downward. To a certain extent, all corrections beyond second order in deformation, shell, and pairing contributions are model dependent. Their accuracy is defined by the degree of sophistication of the theoretical scheme used to estimate them, like particle-number projection, projection of the total angular momentum, two-particle interaction used, etc. The amplitude of the quadratic term in deformation is, however, rather well defined by the liquid drop model only.

In order to have an idea about the role of higher-order terms, in the last column of each table we included also the total energies calculated, using a sixth-order formula in β due to Swiatecki.[13] One must not take these numbers too seriously, since the relation between the quadrupole moment and β is not any more a linear one in such a case, even though we used it implicitly, and also one cannot expect the simpler formula (1) derived by Bertsch to ensure a good estimate of the positions of level crossings. As one sees, the higher-order terms in β correspond to a certain softening of the deformation energy for large deformations. It is not obvious to us that such large deformations can be accurately described in a Hartree-Fock

calculation in a limited spherical basis, which can explain why the deformations for large numbers of particle-hole states are so different in HF and LDM calculations. The energies agree much better, which can be attributed to the fact that the HF method gives a variational estimate of the energy. This will not ensure that the wave functions will be accurately reproduced in a HF method.

A comparison between the liquid drop mass energy formula and the Hartree-Fock results is perfectly in place, since the last has been shown to reproduce the first accurately,[14] when using the Skyrme interaction. One may think of performing a cranked Thomas-Fermi calculation for these nuclei and in this way to "reproduce" the liquid drop energies for these deformations. In our opinion, such a calculation is unlikely to change the conclusions which one can draw from the preceding estimates. If one will consider corrections in $\hbar$ up to fourth order, as M. Brack *et al.*[14] did, practically the only contribution to the total energy left unaccounted for will be due to shell corrections. In order to make the calculations easier, one can first do a "standard" extended Thomas-Fermi calculation[15] and, if desired, include the higher-order terms perturbatively. Next, one can use the Thomas-Fermi density in order to define the Hartree-Fock potential and in this field compute the single-particle wave functions. As shown by Bohigas *et al.*,[15] such single-particle wave functions are practically identical to the Hartree-Fock ones.

We would like to make one more comment concerning the deformability of the Fermi sphere in a real nucleus. The qualitative analysis of Hill and Wheeler[5] and Bertsch[9] was done within the Fermi-gas approximation. However, one can expect a contribution to the stiffness of the Fermi sphere from the interaction term too, due to the finite range of the latter. In the Skyrme force, this is accounted for through the so-called velocity-dependent terms, which in turn lead to a renormalization of the nucleon mass inside the nucleus.[16] For most Skyrme sets, the effective nucleon mass in nuclear matter is roughly between 0.6 m and 0.9 m, where m is the free nucleon mass. In this way one models with a zero-range force the effects of a finite-range interaction. Since the effective mass is smaller than the free nucleon mass (this is true at least for the Hartree-Fock approximation with the Skyrme interaction, which was used in Refs. 1–3), the corresponding local Fermi energy is higher in nuclear matter than in a Fermi gas of the same local density, which will make the Fermi sphere stiffer. One can fairly well expect that the np-nh states found in Refs. 1–4, if they are optimal, must be characterized by a spherical Fermi surface.

As one can see from our simple estimates using the liquid drop model, the deformation energy increases mainly parabolically with the number of particle-hole excited pairs. Higher-order terms in β do not lead to dramatic changes, except for very large deformations in the case of ^{16}O. Shell effects and pairing are completely neglected by us, but we do not expect it to modify largely the main trend. Shell effects are present in a HF calculation and one has to have this in mind when comparing the HF with LDM results. Shell corrections can lead to the appearance of "yrast traps" and therefore to even lower excitation energies in some cases. Pairing can play a major role in lowering even more the excitation energies of certain states. This can lead to a near degeneracy of states with significantly different deformations, and one sees such effects in the calculations of Zamick *et al.*[3] One cannot expect to reproduce such fine effects within a liquid drop model approach. However, mass formulas including A, $A^{2/3}$, $A^{1/3}$, and A^0 terms seem to be able to reproduce the total energy of nuclei extremely accurately[12,17] and the significant lowering of the potential energy for large deformations, which can be generically thought of as np$-n$h excitations, can be understood quite simply within the LDM.

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