Nuclear Shell Structure in the Light of Quark Theory

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Realizing that the internal structure of nucleons undergoes appreciable changes through embedding into nuclear matter the finite nucleus is considered from the outset as a correlated system of quarks. As an appropriate approximation scheme we introduce an extended bag model, i.e. a bag with nuclear radius containing all 3n quarks of the n-nucleon system. As the direct interaction we choose a SU(3)-invariant generalized pairing force which is supposed to contain the major effects of the more general term. As a result of the calculations containing a.o. a rigorous diagonalization of the total Hamiltonian, the characteristic properties of the conventional (nuclear) shell structure are reproduced: The spin orbit splitting appears now as a property of the relativistic single quark states, and the independent nucleon states are represented by correlated 3-quark-clusters. In addition, the nuclear radius law follows directly from a normal value of the vacuum pressure.

1. Introduction

There is, by now, definite evidence that the inner (quark-)structure of the nucleon is essentially changed through its embedding into nuclear matter: A recent CERN-experiment showed this effect with the help of deep inelastic µ-scattering on Fe [1]. On the other hand, this fact is also supported by theoretical arguments: If the structure of the free nucleon is described with the help of a so-called bag model – we take here the example of the MIT-bag [2, 3] – it turns out, as well-known, that the corresponding radius $R$ is of the order of the average distance of the nucleons in nuclear matter. This means that an overlap and hence a deformation of the original structure cannot be prevented. Another (tentative) argument follows from a detailed boson theoretical calculation of the binding energy of nuclear matter: It turns out that a main part of the binding stems from a so-called block-diagram, i.e., a genuine 2-pion exchange in relation to the inner excitations (J-resonance) of the nucleon. In this way a relatively strong admixture of $J$-states is produced which again corresponds to a change of the inner structure [4]. (This fact is to some extent similar to the well-known polarization effect in chemical binding.) From a more general viewpoint one might thus say that a finite nucleus should be visualized as a correlated system of 3n quarks rather than an $n$-nucleon system. Therefore, the question arises whether there is any hope to tackle the problem of nuclear structure directly from such a comprehensive quark theoretical viewpoint. The scope of this paper is to give a partial answer to this question: It will be shown that the characteristic nuclear properties connected with conventional shell structure are obtained in a natural – if not simpler – way by starting directly from this enlarged scheme. At the same time it will be realized that the new quark structure exhibits characteristic correlations which may be interpreted as strongly deformed nucleons within nuclear matter.

The first step of our work consists in the introduction of a suitable approximation scheme for this new 3n-quark (fermion) system. According to various well-known examples (atomic and nuclear shell structure, solid state physics) the following method is widely used: In a lowest approximation the fermions are supposed to be independent but under the influence of a common average potential. As far as the low-lying states are considered (this is, in fact, mostly the case) one starts with a compactly filled shell and introduces the direct interaction as an additional, not necessarily small term in the Hamiltonian. The practical success of this enormous simplification stems from the fact that, through the Pauli principle, the effect of the direct interaction is strongly reduced. Within this frame we try a similar scheme for the nucleus as a system of quarks which are now moving independently in a new kind of average potential: It appears natural to replace this

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"formal" potential by the well-known surface conditions successfully introduced in the MIT-bag model for the nucleons, i.e. for the 3-quark system. At the same time, we assume again the existence of a characteristic surface pressure \( B \) [2] (supposed to be due to the gluons of the degenerate QCD vacuum [5]) in order to provide an equilibrium against the inner pressure of the quarks. In short, our model consists of the assumption that the spherical finite nucleus could be considered as an "overall" bag, i.e. a bag with 3\( n \)-quarks and a radius equal of nuclear dimension. The decisive part of this scheme consists, however, in the introduction of the direct interaction between the quarks (we will introduce a simplified expression which is practically uniquely determined through general principles) and the corresponding exact diagonalization of the total Hamiltonian of the system. Although this model looks at first sight very different from the conventional nuclear shell model, it will be shown that the characteristic experimental properties remain unchanged.

2. The Quark Model for the Nucleus

True to our program the main assumptions of the MIT-bag [2, 3] for light hadrons are taken over into the "overall" nuclear bag: We thus have independent (non-strange) quarks described by the (relativistic) Dirac spinors \( \psi_{kT} \), which contain indices for colour (\( k = 1, 2, 3 \)) and flavour (\( \tau = \pm 1/2 \) or up/down) and have to satisfy the characteristic boundary condition on the spherical surface with nuclear radius \( R \); in addition we have to fulfill the fundamental condition about vanishing total colour of the system. The only differences are thus the choice of \( R \) and the fact that we now have 3\( n \) quarks which will occupy also levels of higher quantum numbers, i.e. in particular higher spins. The equation determining \( \psi_{kT} \) reads (with the quark mass \( m \)):

\[
(z \cdot p + \beta m) \psi_{kT} = \varepsilon \psi_{kT}, \tag{1a}
\]

for \( x < R \), together with the boundary condition for \( x = R \),

\[
x \cdot x / x \psi_{kT} = i \beta \psi_{kT}. \tag{1b}
\]

The first task is the calculation of the single-quark spectrum (\( \varepsilon \)) defined by this system as function of the radius \( R \) and the quark mass \( m \).

Before looking in the details of this spectrum it is important to check the behaviour of the total energy \( E \) (defined as the sum of the occupied single-particle levels \( \varepsilon \)) as a function of \( n \) (for 3\( n \) quarks) and \( R \). It turns out that the characteristic equilibrium condition of the MIT-model, namely [2]

\[
-\frac{\partial E}{\partial R} = 4 \pi B R^2, \tag{2}
\]

where \( B \) represents an appropriate value for the "universal" outer pressure due to the (degenerate) vacuum, leads for all values of \( n \) and a suitable choice of the quark mass \( m \) in reasonable approximation to the well-known radius law for spherical nuclei, i.e. \( R \approx 1.3 n^{1/3} \) [fm]. It is, in fact, important to realize that \( B \) may be assumed to be approximately constant all over the periodic table. At the same time, our \( B \) differs very little from the value used in the MIT-nucleon bag [3]. With \( m = 270 \) [MeV] we obtain for \( B : B^{1/4} = 127 \) [MeV] (against \( B^{1/4} = 100 \) [MeV]). For this reason formula (2) represents in a most natural way the constancy of nuclear density (saturation) which, by now, appears related to the vacuum pressure \( B \).

We should mention that Eq. (2) is slightly too complicated for the practical determination of \( R \); we use, therefore, the approximate relation

\[
-\frac{\partial E}{\partial R} \approx \frac{1}{R} E \tag{3}
\]

(which is strictly correct for massless quarks) in order to convert (2) into the form

\[
E(n, R) = 4 \pi B R^3 \tag{3}
\]

which holds, of course, only for the equilibrium value of \( R \).

In a next step the single quark spectra (\( \varepsilon \)) are looked at in connection with the corresponding spectroscopic assignments, i.e. the values of angular momentum \( j \) and of parity (the combination of both defines the orbital angular momentum \( l \)). Choosing for \( m \) a value between 200 – 300 MeV it turns out that this spectrum is practically identical with the well-known Mayer-Jensen level scheme of conventional nuclear shell structure. This amounts to say that the characteristic (half phenomenological) spin orbit coupling term of the original non-relativistic model is now replaced by a relativistic effect of the Dirac Eq. (1a) in relation to the fundamental surface condition (1b). (It was checked that a generalization of this condition by a position-dependent
mass $m(r)$ of the quarks might lead even to a more accurate representation of the conventional scheme.) If these quark levels are compactly filled according to the Pauli principle one thus obtains in a natural way the closed (double-magic) shells. It is most important to realize that the fundamental condition of vanishing total colour is automatically satisfied in this case. On the other hand, the situation is fundamentally different in the case of open quark shells: Even if the condition about vanishing colour is taken into account, the remaining degeneracy of all possible $3^n$ quark states is still (due to the additional degrees of freedom) by far too large with respect to the nuclear case which corresponds, of course, to the empirical facts. On the other hand, it is easy to construct quark states which in fact exhibit the properties of the expected nuclear states: They form, however, only a small subspace. It is thus clear that the introduction of a direct interaction between the quarks (which plays an important role already in the original bag model) represents a decisive step: It will split this high degeneracy and should thus single out the expected special (nuclear) states as those with lowest energy.

3. The Direct Interaction between the Quarks

The main part of this work consists, in fact, in the introduction of a suitable quark-quark interaction: Realizing that QCD does not yet provide a rigorous expression and that the problem could by no means be treated in an exact way if this interaction is of a general type, we make a decisive simplifying assumption: We assume that our interaction should have the well-known character of a pairing force and that it should satisfy the fundamental principle of SU(3)-invariance. The first assumption is a natural consequence of the fact that the range of the direct interaction is small with respect to the dimension of the system. This argument was, in fact, successfully applied in conventional nuclear structure as well as in superconductivity where it also plays a decisive role; it amounts to say that the pairing matrix elements of the true interaction have an overwhelming influence and that the remaining part may be treated as a perturbation.

If we introduce for the moment the additional simplifying hypothesis that the interaction should act only between quarks within a given $j$-shell we are led to the following expression $P_j$:

$$P_j = -g_j \sum_{i=1}^{3} A_i^* A_i,$$

where $g_j$ are the coupling constants, $a_i(m, \pm 1/2)$ represents the annihilation operator of the state specified by the colour indexes $i$, the magnetic quantum number $m$ and the flavour index $\tau$ with the two values $\tau = \pm 1/2$.

It is readily seen that this force acts on pairs of quarks which are coupled to total angular momentum zero and, at the same time, (through the totally anti-symmetric $\varepsilon$-symbol) to a colour antitriplet state. It was important to realize that this expression is (apart from just one different, but inappropriate choice which contains a coupling to a colour sextet state) uniquely determined by our two assumptions.

Although our force $P_j$ looks rather different from the expression used so far in the MIT-bag model for the nucleon, it has been checked that its action within the 3-quark system yields quite similar results: In fact, a detailed calculation showed [6] that the spectrum of excited states induced by our term agrees to some extent with the experimental values, provided that $g_j$ is chosen in an appropriate way (for $j = 1/2$). It turns out that $g_j$ is so large, that perturbation theory fails. Hence we are confronted with the problem of an exact diagonalization of the total Hamiltonian $H$ of our quark system which now contains the interaction term $P_j$.

More specifically we consider now a core of completely filled shells containing $3n_c$ quarks and a last shell with index $j$ filled partially by $3n_j$ quarks. Thus the total number of quarks is $3n = 3n_c + 3n_j$ and $H$ has effectively the form:

$$H = E_c + 3n_j \varepsilon_j + P_j \equiv H_0 + P_j,$$

where the core energy $E_c$ can be treated as a constant. It is important to remark that we have to single out from the very beginning the eigenstates which satisfy the additional fundamental condition of vanishing total colour because only such states are physically relevant.

The explicit (and exact) diagonalization of $H$ (for arbitrary values of $n_j$ and $j$) is now carried
through with help of rather sophisticated group-theoretical methods [6] of which we will give here just a short survey.

4. The diagonalization of the total Hamiltonian

The general $N_r$-quark eigenstate of the unperturbed Hamiltonian $H_0$ containing $N_j$ quarks within the open $j$-shell is written in the following way:

$$|\psi\rangle = \prod_{r=1}^{N_j} a_{\pi}^{\ast \pi_r} |0\rangle;$$

$a_{\pi}^{\ast \pi_r}$ and $a_{\pi}$ represent the emission and absorption operators, respectively, where the index $i$ stands for colour (as before) whereas $\pi$ stands for the index pair $(m, \pm 1/2)$ of magnetic and isospin quantum number and the subindex indicates the various quarks. According to our program the first task is to single out the states of vanishing total colour: starting with the simplest example we consider the operator

$$A^+(\pi, \beta, \gamma) = \sum_{i,k,l} e_{ikl} a_{\pi}^{\ast \pi_i} a_{\beta}^{\ast \pi_k} a_{\beta}^{\ast \pi_l}. \tag{6}$$

When applied to the vacuum, this operator produces a 3-quark state with total colour zero (in particular, when we restrict ourselves to the lowest shell ($S_{1/2}$), we produce in this way the nucleon and the $J$-particle).

For a general value $n_r$, a natural colour-free 3 $n_r$-quark states $|\psi\rangle$ is obtained by the product operator; i.e.

$$|\psi\rangle = \prod_{r=1}^{n_r} A^+(\pi_r, \beta_r, \gamma_r) |0\rangle. \tag{7}$$

Now, the important point of this construction lies in the fact that this expression yields all possible colour-free states, provided that the $3n_r$ single particle indices $\pi_r, \beta_r, \gamma_r, ((r = 1, \ldots, n)$ are varied arbitrarily; we thus proved that expression (7) exhausts all possibilities.

In a next step a fundamental group-theoretical property of our colour free states (7) is proved. They form, in fact, the representation space of a well-defined irreducible representation of the special unitarity group $SU(N)$ with $N = 2(2j + 1)$. The infinitesimal elements of this group act in a natural way on our states by means of the following operators:

$$\tilde{d} = \sum_{\pi,\beta=1}^{N} d_{\pi \beta} \sum_{i=1}^{3} a_{\pi_i}^{\ast \pi_i} a_{\beta_i}^{\ast \beta_i}. \tag{8}$$

The numbers $d_{\pi \beta}$ are the components of an anti-hermitian and trace-free matrix $d$, i.e. $d^{\ast} = -d$ and $trd = 0$. Note that the linear map $d \to \tilde{d}$ yields a representation of the Lie algebra of $SU(N)$ which, by construction, commutes with the colour rotations. It thus follows that this representation, which is defined on all quark-states, restricts to a representation on the colour-free states alone. The decisive point is that it acts, in fact, irreducibly on this space and may, therefore, be completely classified by its maximal weight. In the notation of [7] we find that it is equal to $3f_{n_r}$. This representation could also be characterized by a Young-diagram with 3 rows and $n_r$ lines; in this form, our result is a straightforward generalization of the characterization of spinless systems in atomic physics within the Russell-Saunders coupling scheme [8].

In a third step we have now to determine the (reduced) symmetry of the total Hamilton $H$ which, of course, does not commute with all the operators given by [8]. In order to describe the infinitesimal operators of this new symmetry we add an additional restriction on the antihermitian matrices $d$ occurring in [8]: If $\tilde{d}$ represents complex conjugation we obtain:

$$\tilde{d} = TdT^{-1},$$

where $T$ is the “linear transformation” defined by

$$T (m, \pm 1/2) = (-1)^{m+1/2 \pm 1/2} |m, \mp 1/2\rangle. \tag{9}$$

While this smaller set of operators $\tilde{d}$ now commutes with the total $H$ it represents at the same time a Lie algebra which is isomorphic to the Lie algebra of the special orthogonal group $SO(N)$, (the last equation states in fact that $\tilde{d}$ is essentially a real antisymmetric matrix). If we restrict the correspondence $d \to \tilde{d}$ (according (8)) to this smaller Lie algebra the action on our states (7), we obtain, of course, a representation of $SO(N)$ but it will now be in general a reducible one; e.g. the space of the states (7) will split in well-defined subspaces which are irreducible with respect to $SO(N)$. On the other hand also the various eigenspaces of $H$ correspond to characteristic representations of the invariance-group $SO(N)$. As a main result it turns out that those are (apart from one exception) also irreducible representations (i.e. $SO(N)$ represents a maximal invariance group). In particular, there is practically a one-to-one correspondence between these eigenspaces and the representation-spaces of $SO(N)$.
mentioned before. These important facts are immediately seen by proving (with the help of an extended computation) that the pairing operator $P_j$ in $H$ may be expressed in terms of the Casimir operators $C_1(N)$ and $C_2(N)$ for the representation (8) of $SU(N)$ and $SO(N)$, respectively:

$$P = -g_j \left[ (N-2) C_1(N) - NC_2(N) + \frac{1}{2N} N_{\text{op}}^2 - \frac{1}{2} N_{\text{op}} \right].$$

(9)

$N_{\text{op}}$ is the number operator and can be replaced by its eigenvalue $3n_j$. (This formula again shows that $SO(N)$ is a symmetry group of $H$.) By now it is clear how we can achieve the exact diagonalization of $H$: We just have to determine explicitly the irreducible components contained in our (reducible) representation of $SO(N)$; acting in the space of colourless states (7). Group-theoretically this means that we have to determine the corresponding maximal weights. In such an irreducible component, $P_j$ and hence $H$, are necessarily diagonal (being sums of Casimir operators!); moreover, we obtain the corresponding eigenvalues of $H$ simply by inserting the eigenvalues of the Casimir operators (these values are readily computed from the highest weights by means of a classical formula [7]).

As a first important result of this procedure we may state that $H$ has the following eigenvalues (in the space of 3 $n_j$-quark states with vanishing colour):

$$E(l_j) = E_{\text{core}} + 3n_j \epsilon_j$$

(10)

$$-g_j(n_j(N+3-n_j) - l_j(N+3-l_j)),$$

where $l_j$ takes on integer values with $0 \leq l_j \leq \min(n_j, N-n_j)$. Recall $SO(N)$ acts irreducibly in each eigenspace (except for $n_j = N/2$, when the corresponding eigenspace splits again into two components). At the same time our construction allows in principal the detailed determination of all eigenstates (in particular the various degeneracies) of $H$.

5. Nuclear Shell Model States in Terms of Quark States

Having determined our energy eigenvalues, we have to discuss now the structure of the corresponding eigenspaces. In fact, it turns out that the energy eigenstates still exhibit a characteristic degeneracy; if we look, however, at the explicit structure of the eigenspace corresponding to the lowest eigenvalue ($l_j = 0$) it turns out as a main result of our analysis that the general properties of these lowest energy states correspond exactly to those expected from the corresponding open shell states (without direct interaction) of the conventional Mayer-Jensen shell model for nucleons, i.e. the same degeneracy and same quantum numbers for the angular momentum and isospin, etc. occurs. As an example the eigenstates for $n_j = 1, l_j = 0$, e.g. three quarks in an open shell read explicitly

$$|\psi\rangle = \sum_{k=1}^{3} a_{\tilde{k}x}^{*} A_{\tilde{k}}^{*} |0\rangle$$

(11)

(compare Eq. (4) for the explicit form of $A_{\tilde{k}}^{*}$).

Recalling that $x$ stands for an index pair of angular momentum $m$ and isospin $\tau$, it is immediately realized that this state (which is $SU(3)$-invariant, compare Eq. (7)) has the correct quantum number of a nucleon in the corresponding shell, e.g. this expression simulates a proton or a neutron with angular momentum $m$. The expression (11) could be visualized as a quark pair ($A_{\tilde{k}}^{*}$) coupled to a kind of valence quark which bears the quantum number of the corresponding nucleon. It might thus be interpreted as the (strongly) deformed quark structure of a nucleon embedded in nuclear matter (note that $|0\rangle$ denotes a closed-shell core). Moreover, the $n_j$-nucleon states in this shell are naturally given by the products of the corresponding operators $j$, setting

$$B_j = \sum_{k=1}^{3} a_{\tilde{k}x}^{*} A_{\tilde{k}}^{*}. $$

these states can be written in the form:

$$\psi = \prod_{i=1}^{n_j} B_{z_i} |0\rangle.$$

It may be directly checked that these expressions are, in fact, eigenstates of $H$, but it is by no means trivial that they yield the full eigenspace of the lowest eigenvalue. This fact represents the major result of our detailed mathematical analysis. [6].

This means that we have, by now, established a perfect one-to-one relation between the lowest states of our quark model and the states obtained by filling in the shells of the conventional structure by independent nucleons (the characteristic operators $B_j$, in Eq. (12) correspond to the emission operators of entire nucleons). Note that all these states are
A degenerate within the framework of this new picture; it appears thus of decisive importance to take, in the course of further developments, an additional interaction between these nucleon substructures into account. In our quark theoretical case this renewed splitting will be automatically obtained by introducing a more refined realistic quark-quark interaction.

Having thus realized the correspondence to conventional shell structure, the question arises how to interpret the large number of high-lying excited states \( E_i \) which are, of course, characteristic for our model. From a comparison with the 3-quark system it follows that all these excitation energies are of the same order of magnitude as the inner excitation of a free nucleon (i.e. \( \Delta \)-excitation). In fact we would like to suggest that these new states are in a certain sense related to those obtained in the conventional structure by the inner excitation of the various nucleons. This hypothesis which needs, however, a further and more detailed analysis, allows an empirical determination of \( g_j \). It turns out that \( g_j \) can be conveniently parametrized in the form \( g_j = 120/(2j+1) \) [MeV]. The parameters of our model are now completely specified and we have checked that nuclear masses and radii are in fact correctly reproduced.

6. Conclusions

The main results of the explicit calculations in the framework of our nuclear bag model are thus the following:

1. The general saturation properties (i.e. the well-known radius law) as well as the characteristic spin orbit splitting of shell structure follow, so to speak, in a natural and most direct way from our relatively simple and intuitive basic assumption. These two facts are by no means trivial: The calculation of the density of nuclear matter (which is equivalent to the determination of the radius) represents, as far as conventional nuclear theory is concerned, an enormous and so far not definitely solved problem: It depends essentially on the explicit (and complicated) form of the NN-force as well as on the introduction of rather refined mathematical approximation schemes (i.e. Bethe-Brueckner theory, with the hole-line expansion or the Fermi-hypernetted-chain approximation scheme). In our case this value is determined directly through the fundamental outer pressure \( B \) in connection with the single particle energies of the occupied quark states. The same situation holds in the case of the spin orbit splitting: In the conventional case the determination of the (phenomenological) single particle \( (L \cdot S)\)-potential also represents a difficult and not definitely solved problem (the corresponding terms in the nucleon-nucleon force which are mainly due to the \( \omega \)-exchange appears not to produce the full amount needed). In the quark theoretical case, again, the splitting follows most naturally as a (relativistic) property of the Dirac equation in connection with the characteristic surface condition.

2. The typical properties of conventional shell structure (including the assignments and degeneracy of the states corresponding to the various shells) are again reproduced in a natural way. In particular, it is seen that the magic numbers are now found as a consequence of the Pauli principle applied directly to the fermion system of quarks. This fact appears of importance for the following reason: In conventional shell structure the nucleons have to be assumed to be exactly identical in order to apply this principle. In view of the fact that the nucleons within nuclear matter are, as we have seen, relatively strongly polarized (some estimates mention a degree of about 7%) [9] this assumption is, in fact, not satisfied. A more detailed analysis of the situation might show that this polarization effect could, so to speak, wipe out the characteristic (and experimentally well established) energy steps of the separation energies at the position of the magic numbers [10]. From a more general viewpoint one might say that these characteristic energy steps could be taken as a hint that the system in question is, in fact, composed by ideal fermions, i.e. the quarks which, therefore, satisfy the Pauli principle exactly [11].

In conclusion it might be mentioned that this model is based on a relatively small number of phenomenological parameters: Mass \( m \) of the quarks, vacuum pressure \( B \) and coupling constants \( g_j \) (supposed to be all of the same order of magnitude). It thus appears of greatest interest to interpret \( B \) from a general quantum chromodynamical viewpoint [5]. On the other hand, the values for \( g_j \) would be obtained from an explicit calculation of the various pairing matrix elements with the help of a more basic expression of the direct quark-quark interaction.
interaction. In the framework of our approach this force acts only through these special matrix elements which are supposed (according to the general principles of pairing theory) to contain the most important part of the complete interaction matrix. In a further development a large number of more general matrix elements must be determined; they might, however, be considered as a perturbative part of the total Hamiltonian. Among many other effects they have to replace the direct nucleon-nucleon interaction of the conventional scheme.

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