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A (ud)-cious model of the proton

Sverker Fredriksson
Department of Physics
Luleå University of Technology
S-951 87 LULEÅ
Sweden
Lulea U.

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Abstract

In collaboration with Svante Ekelin and Göran Rangne at the Royal Institute of Technology in Stockholm, I have tried to solve, by variational methods, the three-quark, QCD inspired hamiltonian of De Rújula et al. The spin-spin coupling gives rise to a bound scalar (ud) diquark with a radius much smaller than that of the proton. The spin forces from the single u quark are, however, strong enough to disturb severely the scalar (ud) system. This results in a substantial fraction of the proton wave function being similar to a normal three-quark system. Thanks to this admixture the proton-to-neutron magnetic moment ratio is well reproduced, something that normally poses a problem to models with small scalar diquarks. These results illustrate the inadequacy of the conventional perturbative treatment of spin forces when analysing hadron quark structure. A unified picture of the role of small diquarks in constituent nucleons and high-energy reactions is promoted.

(**judici'ous** *a.* wise; prudent; showing discrimination)

1 Introduction

The most widespread method to analyse the influence of quark colour forces on the properties of nucleons is to find approximate solutions to the non-relativistic hamiltonian [1,2,3]:

$$H = H_{conf} + H_q + H_{ss} + H_{coul} + H_{rp} + H_{ls} + H_{rs}, \tag{1}$$

where

H_{conf} is the overall confining potential energy,

$$H_q = 3m - \frac{1}{2m}\sum_i \Delta_i ,$$

$$H_{ss} = \frac{2\pi\alpha_s}{3m^2}\sum_{i>k} \Delta V(r_{ik})\left(1 + \frac{8}{3}\mathbf{S}_i\cdot\mathbf{S}_k\right),$$

$$H_{coul} = -\frac{2\alpha_s}{3}\sum_{i>k} V(r_{ik}),$$

$$H_{rp} = -\frac{\alpha_s}{3m^2}\sum_{i>k} V(r_{ik})\left(\nabla_i\cdot\nabla_k + \frac{\mathbf{r}_{ik}\cdot(\mathbf{r}_{ik}\cdot\nabla_i)\nabla_k}{r_{ik}^2}\right),$$

$$H_{ls} = -i\frac{\alpha_s}{3m^2}\sum_{i>k}\frac{1}{r_{ik}} V'(r_{ik})[\mathbf{r}_{ik}\times(\nabla_k - \nabla_i)]\cdot(\mathbf{S}_i + \mathbf{S}_k),$$

$$H_{rs} = -\frac{2\alpha_s}{9m^2}\sum_{i>k}\left[V''(r_{ik}) - \frac{1}{r_{ik}} V'(r_{ik})\right]\left[\mathbf{S}_i\cdot\mathbf{S}_k - 3\frac{(\mathbf{r}_{ik}\cdot\mathbf{S}_i)(\mathbf{r}_{ik}\cdot\mathbf{S}_k)}{r_{ik}^2}\right].$$

Here $\mathbf{r}_{ik} = \mathbf{r}_i - \mathbf{r}_k$ and $r_{ik} = |\mathbf{r}_{ik}|$, where $\mathbf{r}_i$ marks the position of the *i*th quark, with spin vector $\mathbf{S}_i$. Furthermore, α_s is the strong coupling constant, m is the (common u and d) quark mass, ∇ is the gradient operator ($\Delta = \nabla^2$), and V is the colour potential. We neglect electromagnetic forces. As this QCD hamiltonian is inspired by quantum electrodynamics one normally sets $V(r) = 1/r$, which leads to the well-known spin-spin factor $\Delta V(r) = \delta(r)$, representing a contact coupling. One then avoids calculational problems by using the SS term only as a first-order perturbation to the free-quark situation, hoping that the effect on the wave function be small. The more complicated last three contributions are usually neglected.

This procedure is, however, not satisfactory as it is obvious that the SS term is the main cause of the rather large proton-delta mass difference of about 300 MeV. Any "perturbative" force that gives a change in energy of more than 30% could be suspected to also influence the quark wave functions to a large extent, and such changes can naturally not be analysed in the framework of a first-order perturbation theory. Also the mixed "rp" force will be shown here to be important, in support of the analysis in [4]. We ignore the terms H_{ls} and H_{rs}, since they vanish in S-wave solutions.

For the last few years we have argued that there are strong empirical indications that the proton wave function is different from that of three weakly interacting quarks confined to a common volume. In a series of publications [5] we have suggested that two of the quarks, one u and one d, in a proton or neutron, are bound into a spin-0 diquark with a radius of only 0.1-0.3 fermi. Other quark combinations form scalar diquarks in strange or charmed spin-1/2 baryons. When trying to support this view by a theoretical calculation based on the QCD hamiltonian (1), it is obvious that a perturbative treatment would be inconclusive. This is probably one of the reasons why the diquark solution has so far not been noted by groups that use (1) for studies of nucleons. For a recent review of diquarks, see [6].

2 The formalism

Let us start the description of the proton by defining quarks 1 and 2 as being the two u quarks, while quark 3 is the d quark. We next pose a restriction on the model by prescribing the d quark to be in a spin-0 configuration with at least one of the u quarks. This requirement can be relaxed, at the cost of a more complicated algebraic analysis. We choose a spin-0 combination because it gives rise to an attractive spin-spin force according to (1), which leads us to believe that nature prefers at least one spin-0 pair in a nucleon (the orthogonal spin structure cannot easily be brushed off in this formalism, because of rather complicated cross terms in the matrix elements).

The basic expression on which to build a proton wave function then reads

$$\Psi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)u_1\uparrow(u_2\uparrow d_3\downarrow - u_2\downarrow d_3\uparrow), \tag{2}$$

with ψ being a spatial wave function in the quark coordinates.

The total proton wave function must be symmetrised in the two u quarks. We do not symmetrise in u and d, because the hamiltonian does not contain any isospin dependence. We get

$$\begin{aligned} |p\uparrow\rangle = {} & [\Psi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3) + \Psi(\mathbf{r}_2,\mathbf{r}_1,\mathbf{r}_3)]\ |u\uparrow u\uparrow d\downarrow\rangle - \\ & - \Psi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)\ |u\uparrow u\downarrow d\uparrow\rangle - \Psi(\mathbf{r}_2,\mathbf{r}_1,\mathbf{r}_3)\ |u\downarrow u\uparrow d\uparrow\rangle. \end{aligned} \tag{3}$$

In order to construct a realistic spatial part of the wave function we start with the factorised form

$$\phi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3) = A\ \exp[-a_1(\mathbf{r}_1-\mathbf{r}_2)^2]\ \exp[-a_2(\mathbf{r}_2-\mathbf{r}_3)^2]\ \exp[-a_3(\mathbf{r}_1-\mathbf{r}_3)^2]. \tag{4}$$

This basic form has several advantages, except for the fact that gaussians are customary for describing particles in relative motion.

First, it leads to analytic expressions for all matrix elements, including the "rp" ones, provided we choose a suitable expression for the term H_{conf} in (1):

$$H_{conf} = k_{conf} \sum_i \mathbf{r}_i^2 - E_0, \tag{5}$$

where k_{conf} and E_0 measure, respectively, the width and depth of the confining potential. Also a linear form leads to (more complicated) analytic solutions.

Secondly, the form (4) is symmetric enough in indices 1,2,3 to give fairly simple algebraic manipulations when relating various matrix elements to each other.

Thirdly, the values of a_1, a_2 and a_3 that finally give the solution to the problem are simple to interpret. The a_2 is related to the mean distance between the u and d quark inside the scalar diquark, a_1 to the distance between the two u quarks and a_3 to the distance between the d quark and the single u quark.

Finally, the expression (4) includes both the possibility of a small (ud) diquark, corresponding to $a_2 >> a_1 \approx a_3$, and that of a normal three-quark state, with $a_1 \approx a_2 \approx a_3$.

Up to here this formalism is about the same as the one I presented four years ago at the first diquark meeting [5]. It gave solutions that represent very small (ud) diquarks, the radius being of the order of 0.1 fm. However, no efforts were done to get correct values for any other observables than the nucleon and delta masses and the proton overall size. It was, for instance, obvious that the proton-to-neutron magnetic moment ratio came out close to -2 instead of the observed value of around -1.5.

The physical reason for this might be that the very small diquark is severely disturbed by attractive spin forces between the d quark in the (ud) and the other u quark. This is due to the fact that also the "non-diquark" ud pair is some fraction of its time in a spin-0 state. The d quark might then "tunnel" out of the genuine diquark and either form a more loosely bound diquark with the wrong u quark, or it might stay somewhere in-between the two u quarks in something like a normal three-quark state.

We have chosen to simulate this situation by extending the spatial wave function to the form

$$\begin{aligned}\Psi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3) = {} & A \exp[-a_1(\mathbf{r}_1-\mathbf{r}_2)^2] \exp[-a_2(\mathbf{r}_2-\mathbf{r}_3)^2] \exp[-a_3(\mathbf{r}_1-\mathbf{r}_3)^2] \\ & + B \exp[-b_1(\mathbf{r}_1-\mathbf{r}_2)^2] \exp[-b_2(\mathbf{r}_2-\mathbf{r}_3)^2] \exp[-b_3(\mathbf{r}_1-\mathbf{r}_3)^2].\end{aligned} \tag{6}$$

The first term in (6) corresponds to what we expect to contain the small (ud) diquark, while the second term contains the possibility of the "false" ud combination or a three-quark component.

We now set out to minimise the matrix element

$$E_{tot} = \langle p|H|p\rangle \tag{7}$$

with respect to the eight parameters A, B, a_1, a_2, a_3, b_1, b_2 and b_3, given that they are related through one normalisation condition ($\langle p|p\rangle = 1$).

Another problem must be solved before a solution can be found. It is obvious that the solution for a singular spin-spin coupling of the type $\Delta V(r) = \delta(r)$ is given by an infinitesimally small (ud) diquark ($a_2 \rightarrow \infty$) and an infinitely strong binding ($E_{tot} \rightarrow -\infty$). This can be seen from the well-known result that the kinetic energy of a gaussian wave function, $\exp(-br^2)$, grows like b (or like $b^{1/2}$ in the relativistic limit), while the matrix element of a negative δ-function goes like $-b^{3/2}$ (in 3 dimensions). Hence $\langle p|H|p\rangle$ has no minimum.

This problem can easily be avoided by choosing the radial part of the spin-spin coupling as

$$\Delta V(r) = (g/\pi)^{3/2} \exp(-gr^2). \tag{8}$$

Here g is a parameter that determines the range of the spin forces. In the limit $g \rightarrow \infty$ one recovers the δ-function. Consequently, we must replace the function V(r) in the hamiltonian with

$$V(r) = \mathrm{erf}(\sqrt{g}\ r)/r, \tag{9}$$

where erf(x) is the error function.

The substitution of the usual Coulomb interaction with the one in (9) is not only a computational necessity, but also a realistic way of simulating asymptotic freedom in QCD, as the Coulomb term no longer diverges when $r \rightarrow 0$. Obviously the solution to the variational problem depends strongly on the choice of the parameter g.

Before computing the various matrix elements

$$E_{..} = \langle p|H_{..}|p\rangle, \tag{10}$$

which sum up to the total energy, we need to fix the centre of mass of the three-quark system. This is done by a factor $\delta^{(3)}(\mathbf{r}_1+\mathbf{r}_2+\mathbf{r}_3)$ in all integrands.

All integrals can now be analytically evaluated with the help of either of these formulas:

$$\int..\int (c_1\mathbf{r}_1^2 + c_2\mathbf{r}_2^2 + c_3\mathbf{r}_1\cdot\mathbf{r}_2 + c_4)\ \exp[-(d_1\mathbf{r}_1^2 + d_2\mathbf{r}_2^2 + d_3\mathbf{r}_1\cdot\mathbf{r}_2)]\ d^3r_1 d^3r_2$$
$$= \frac{3}{4}\pi^3(2c_1d_2 + 2c_2d_1 - c_3d_3)(d_1d_2 - d_3^2/4)^{-5/2} + \pi^3 c_4(d_1d_2 - d_3^2/4)^{-3/2} \qquad (11a)$$

and

$$\int_0^\infty \exp(-ar^2)\ \mathrm{erf}(\sqrt{g}r)\ (Ar + Br^3)\ dr =$$
$$= \frac{1}{4a^2}\left(1 + \frac{a}{g}\right)^{-3/2}\left[2aA\left(1 + \frac{a}{g}\right) + B\left(2 + \frac{3a}{g}\right)\right]. \qquad (11b)$$

Within the same general scheme we can also compute the mass of the spin-3/2 Δ^{++}. As it does not contain any scalar two-quark combination we can use the much simpler one-parameter spatial function

$$\Psi_\Delta(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3) = A_\Delta\ \exp[-a_\Delta(\mathbf{r}_1^2 + \mathbf{r}_2^2 + \mathbf{r}_3^2)]. \qquad (12)$$

The total Δ^{++} wave function then becomes

$$|\Delta^{++}\uparrow\rangle = \Psi_\Delta(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)|u\uparrow u\uparrow u\uparrow\rangle. \qquad (13)$$

All in all, we now have ten free parameters in the two test wave functions, namely A, B, a_1, a_2, a_3, b_1, b_2 and b_3 for the proton and A_Δ and a_Δ for the Δ^{++}. Except for two normalisation conditions they will all be given by the minimising of $\langle p|H|p\rangle$ and $\langle\Delta^{++}|H|\Delta^{++}\rangle$.

Also the hamiltonian contains unknown parameters:

- m = the quark mass
- α_s = the strong coupling constant
- g $\Leftrightarrow$ the range of the spin-spin potential
- k_{conf} $\Leftrightarrow$ the width of the confining potential
- E_0 = the depth of the confining potential

These five parameters are constants of nature and must be derived from fits to measured quantities. It is suitable to choose the following data:

- the proton mass (938 MeV)
- the Δ^{++} mass (1232 MeV)
- the proton (charge) radius squared (20 GeV^{-2})
- the neutron charge radius squared (- 0.14 times that of the proton)
- the proton-to-neutron magnetic moment ratio μ_p/μ_n (- 1.46)

3 Results (preliminary)

The analytic expression for the proton energy is tremendously complicated and cannot be written down explicitly here. The spin-spin and "rp" terms, for instance, would each fill several pages. In the actual computation we have let the computer start from the integral formulas (11) and limited the algebraic manipulations to finding the analytic expressions for the parameters c_1, c_2 ... in each energy term separately.

We have found clear variational minima in the expression for the proton energy. The results are still preliminary, because we have not looked yet for the best fits to all observables mentioned above, but rather stopped after achieving reasonable values for most of them.

The following qualitative trends have been found in the "minimal" wave function of the proton:

The first term in the spatial wave function corresponds to a very small scalar (ud), with a radius around 10% that of the proton.

The second term corresponds to a situation where the d quark is fairly far apart from both u quarks, with the u quarks most of the time on opposite sides of the d. This looks like a conventional three-quark state.

The two terms mix in the proportion B/A ≈ 0.3, which means that the three-quark component is more frequent than the quark-diquark component.

The proton and delta masses as well as the proton radius are easy to fit, while the magnetic moments require some fine-tuning. The neutron charge radius poses a problem. We have still not been able to get closer than -0.2, compared to the empirical number -0.14 quoted above.

As far as the parameters are concerned we get the following (approximate) results

for those in the hamiltonian:	for those in the wave function:
$m = 300$ MeV	$a_1 = a_3 = 0.01$ GeV^2
$\alpha_s = 0.3$	$a_2 = 0.8$ GeV^2
$g = 3.5$ GeV^2	$b_1 = 0.0035$ GeV^2
$k_{conf} = 0.004$ GeV^4	$b_2 = b_3 = 0.016$ GeV^2
$E_0 = 294$ MeV	$B/A = 0.3$

The energies that sum up to the proton mass are

$E_q = 3m + 594$ MeV = 1494 MeV
$E_{conf} = -116$ MeV
$E_{coul} = -136$ MeV
$E_{ss} = -154$ MeV
$E_{rp} = -154$ MeV

4 Discussion and conclusions

The diquark parameter a_2 is about 80 times bigger than a_1 and a_3, showing that the scalar diquark is about nine times smaller than the other two-quark pairs. We have not yet tried to derive the size of the (ud) diquark in a fictitious situation where it is not disturbed by a third quark. It might then be even smaller.

The parameter b_1 is about four times smaller than the b_2 and b_3, showing that the distance between the two u quarks in the three-quark component is twice that between the d quark and either u quark. This supports the picture of the d quark staying at the proton centre of mass, with the u quarks orbiting on opposite sides. One might argue that the two u quarks are "pushed" apart due to the Pauli principle.

The proton is not very often in a quark-diquark state - just about 20% of the time. However, the best-fit parameter B/A is rather sensitive to the fine-tuning of other parameters, and might change if we try to get a better fit to the neutron charge radius by manipulating the values of, for instance, m and α_s.

The energy values listed above look realistic in the sense that they are fairly non-relativistic. This might be an artefact, however, since very high kinetic and binding energies are expected inside such a small scalar diquark, and the overall values come out small only because the corresponding component of the wave function is small. The hamiltonian (1) is essentially non-relativistic, which means that the precise value derived for the diquark radius cannot be trusted.

Another drawback of the formalism is that we do not know how close the solution is to the true wave function. Naturally, the situation is improved compared to the one presented in [5], with only the A component in the test function. But there are many ways to extend that simple approach into something more realistic. One would be to add also a third component to the wave function where the d quark is not in spin 0 with any of the u quarks.

A third problem is that the A and B components in the spatial wave function are not orthogonal. There is a considerable overlap between the two, which is hard to interpret. One might ask what the orthogonal state, compared to our

solution, could be, and one answer might be the Roper resonance. However, it is not clear that an approximate variational solution to a quantum mechanical problem has orthogonal states which approximate physically observable states. In this case, the Roper resonance would be a state which is frequently in a quark-diquark configuration and less often in a three-quark component. This does not sound realistic.

Finally, I would like to compare the picture emerging here with the one suggested by Don Lichtenberg [7] in his concluding talk at this meeting and with other paradoxes and problems that arise because diquarks sometimes look small and sometimes big.

Obviously, the current formalism treats the proton wave function as a function of the coordinates of the three quarks. As pointed out by Don and by Pire [8], a small distance between two quarks does not mean that the diquark itself need to be small, because the quark pair is dressed-up with gluons and virtual quark-antiquark pairs. It can still have a radius of, say, 0.6 fm even if the two-quark distance is only 0.1 fm, showing just that the radius of a dressed-up quark is around 0.5 fm. If, in addition, there is a considerable three-quark admixture in the proton, the effective scalar (ud) wave function might well look like the one in Don's Fig. 4.

This also solves the problem, shared by all models with small diquarks, that a scalar diquark cannot be smaller than the pion, because the pion is kept together by spin forces that are stronger than those inside a scalar (ud) diquark. However, also the pion radius is a measure of the size of the dressed-up quark-antiquark pair rather than of the quark-antiquark distance. Hence a "naked" scalar (ud) diquark can be very small indeed without being in conflict with the measured size of the pion. Similar arguments were presented a few years ago also by Betman and Laperashvili [9], after they had found that 't Hooft instantons give rise to small scalar diquarks.

The picture promoted does not only aim at a unified quark-diquark model of the nucleon but also at understanding high-energy reactions where small diquarks are probed on their own. Examples are high-p_T hadron reactions and e^+e^- annihilation. Both provide opportunities to give a quark pair a high momentum transfer and therefore to probe the size of a naked quark pair with the cloud shaken off. It is extremely encouraging that the high-p_T proton production from the CERN ISR can be explained [10] as the scattering of a scalar diquark with a radius of 0.1-0.2 fm and an admixture in the proton wave function of 15-30% as compared to a three-quark state. This is fully in line with the (preliminary) numerical results given here (those data can also be explained with a higher admixture of small diquarks [11] together with other input assumptions). Also a collection of e^+e^- data at not-too-high energies (below 10 GeV) can be explained with very small scalar diquarks of various flavours [12]. A more speculative playground for small diquarks is inside a diquark-dominated QCD plasma, maybe in a supernova [13,5].

In conclusion, we have found a variational solution to the three-quark hamiltonian of De Rújula et al., which shows that there is a very small scalar (ud) diquark hidden inside nucleons. It is severely disturbed by the presence of the third quark. This leads us to a unified picture for the role of small diquarks for both baryon static properties and high-energy hadron reactions.

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