Parity Doublets in Quark Physics

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There are numerous examples of very nearly degenerate states of opposite parity in molecular physics. The ammonia maser is based on one such doublet. Theory shows that these parity doublets can occur if the nuclear shape in the molecule is reflection asymmetric because the time scales of the shape and the electronic cloud are well separated. Parity doublets occur in nuclear physics as well for odd $A \sim 219-229$. We discuss the theoretical foundation of these doublets and on that basis suggest that parity doublets should occur in particle physics too. In particular they should occur among baryons composed of cbu and cbd quarks. [S0031-9007(96)02062-5]

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In molecular physics, low energy excitations are rotational bands stacked on vibrational energies E_n (see, for example, Ref. [1]). For a molecule with moment of inertia I, they have energies $E_n + J(J+1)/2I$ with the angular momentum J assuming successive values. The separation $E_{n'} - E_n$ of vibrational excitations is much larger than rotational energies. Now if the levels (n, J) for given n and J are nondegenerate (but for angular momentum degeneracy), then one of the transitions $(n', J) \rightarrow (n, J)$ or $(n', J \pm 1) \rightarrow (n, J)$ would be forbidden in the dipole approximation by parity conservation, and the corresponding spectral line would be weak. This is so because in this scenario, states of successive J and the same n differ in parity. This is seen, for example, in the spectrum of C_2H_2 [2].

But there are molecules like C_2HD and NH_3 where there is no such intensity alternation [2]. Chemists interpret this result as an indication that there is a pair of approximately degenerate levels of opposite parity sitting at each n and J. These parity doublets have also been directly observed for some molecules like NH_3 [2], the ammonia maser being based on just such a doublet [3].

In nuclear physics, there is evidence for pear-shaped nuclei in the range odd $A \sim 219-229$ [4,5]. Parity doublets have been found for these nuclei too [4–7], although their level separation is not small [4,5].

Parity doublets occur if the shape is reflection asymmetric. It thus seems that reflection-asymmetric shapes can lead to approximately degenerate parity doublets under favorable circumstances.

There is good reason to regard this physical phenomenon as truly remarkable. The effective theory of these doublets would be (approximately) U(2) symmetric even though there is no trace of such a symmetry in the microscopic Hamiltonian. This U(2) furthermore mixes states of differing parity. So what we have here is the striking emergence of spontaneous chiral symmetry. And that is not all. Below we shall indicate the theory of these doublets (and elsewhere [8] more thoroughly develop it) and point out their significance for such an apparently remote topic as topology change in quantum gravity. But our principal concern in this paper is with a different subject. The above phenomenon has specific implications for the phenomenology of particle and especially heavy quark physics, and it is the latter that we focus on in this Letter.

Parity doublets occur typically in systems with two differing time scales. For molecules, the fast variables are electronic and the slow ones are nuclear. For nuclei, they are the intrinsic and the rotational degrees of freedom. These systems are amenable to treatment in the Born-Oppenheimer (B-O) approximation [1]. In this approximation, there is a simple and vivid manner to understand the mechanism behind these doublets. Thus, consider, for example, a molecule like C_2HD [1,2]. It is a linear molecule with D at one end, and can be approximated by a unit vector $\vec{n}$ (parallel to the molecule with the tail at D) when finding the rotational levels. The electronic Hamiltonian $\mathcal{H}_F$ in the B-O approximation is diagonalized by treating $\vec{n}$ as fixed. Now the system as a whole is rotationally invariant, so for fixed $\vec{n}$, $\mathcal{H}_F$ is invariant under rotations about the axis $\vec{n}$. If $\vec{J}_F$ is the fast variable angular momentum, an eigenstate of $\mathcal{H}_F$ can be associated with a definite value of $\vec{n} \cdot \vec{J}_F$. It need not be zero, indeed it will not be so for an odd number of electrons, as then no component of $\vec{J}_F$ has eigenvalue zero. But $\vec{n} \cdot \vec{J}_F$ reverses under parity $\mathcal{P}$, so there is another state with the opposite value of $\vec{n} \cdot \vec{J}_F$ when the latter is nonvanishing. When we pass beyond the B-O approximation, the exact Hamiltonian $\mathcal{H}$ mixes these levels, thus creating mutually split even and odd energy eigenstates.

Now there are, of course, many shapes in nature. The configuration space of a shape is just an orbit of the rotation group [9,10]. It is thus $SU(2)/H$ for a subgroup H of SU(2). The molecule is an arrow only if $H = U(1)$. Elsewhere [10], the quantum theory of a generic shape was treated in detail, and it was effectively shown that parity doublets can occur if the shape lacks reflection symmetry even if $H \neq U(1)$. (Cf. the section on heavy mesons, Skyrmions, and monopoles. The content of that paper is best combined with [8] to reach this conclusion rigorously.) Let us give an example. If the molecule

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is a pyramid with the symmetry $Z_{2N} \subset SU(2)$ around an axis $\vec{n}$, then the eigenstates of $\mathcal{H}_F$ can be associated with definite values of $\exp[(2\pi i\vec{n} \cdot \vec{J}_F)/N]$. It determines helicity $\vec{n} \cdot \vec{J}_F$ only mod N. Under parity, $\exp[(2\pi i\vec{n} \cdot \vec{J}_F)/N] \to \exp[(-2\pi i\vec{n} \cdot \vec{J}_F)/N]$, and hence there are parity doublets unless $\exp[(2\pi i\vec{n} \cdot \vec{J}_F)/N] = \pm 1$. Thus an N-fold axis, defining only helicity mod N, can also lead to parity doublets.

Parity doublets are also time-reversal ($\mathcal{T}$) doublets [10]. That is because $\mathcal{T}$ reverses $\vec{J}_F$ and hence $\vec{n} \cdot \vec{J}_F$, just as $\mathcal{P}$ does. But we recall that there could be $\mathcal{T}$ doublets both with trivial parity $+1$, as it happens with staggered conformations [10].

Baryon physics.—All this could be of concern also to a particle physicist. Thus tentatively regarding u and d as light and the remaining quarks as heavy, the following potential parity-doubled baryon states come to mind: (1) scu, scd, (2) cbu, cbd, and (3) btu, btd. But there are two important issues to be addressed before we can entertain the conjecture of parity doublets among these combinations, namely, (1) the existence of two well-separated time scales, T_{slow} and T_{fast} associated with the heavy and the light quarks, and (2) the relative magnitude of T_{slow} and quark lifetimes τ. Item (1) is, of course, the basis of canonical B-O approximation while (2) is new. It is just that the entire approximation scheme can break down if a quark decays too fast. It is thus necessary to check that the lifetimes of quarks are much longer than the dynamical time T_{slow} in the problem. Below we outline how we treat (1) and (2) and then summarize the pertinent numbers in tables.

Item (1): Assuming that the distance between the two heavy quarks is of the order of 1 fm, we will estimate T_{slow} as follows. If I is the moment of inertia of the heavy quark pair, and J its angular momentum, then $T_{\text{slow}} \approx 2\pi I/J \approx 2\pi I = 2\pi\mu R^2$, where μ is the reduced mass and $R \approx 1$ fm is the relative separation of the heavy quarks. We will estimate μ and T_{slow} using constituent quark masses, as it is more appropriate than using current quark masses.

As for T_{fast}, by the uncertainty principle, the momentum p of a fast quark is $\approx 1/R$. It is also $mv/\sqrt{1 - v^2}$ for a quark of mass m. In this way, we can find $T_{\text{fast}} \approx 2R/v$.

Item (2): Quark lifetime scales as the fifth power of the mass. Crude estimates for τ good enough for us can be obtained by scaling muon lifetime.

Constituent quark masses and their lifetimes are shown in Table I, while numbers for T_{slow} and $T_{\text{slow}}/T_{\text{fast}}$ are shown in Table II.

From the tables, one sees that cbu and cbd baryons are the best candidates to search for parity doublets. Since J_F, the total angular momentum of the light quark, is necessarily half-integral, we expect that parity doublets will occur. In addition to parity doublets, the model, of course, predicts normal rotational excitations. Their splitting would be of the order of $1/2I \simeq 100$ MeV and can be looked for experimentally. It is difficult to estimate the energy difference between the parity doublets. It could be of the order of 100 MeV (that is, of the order of rotational excitation energies as in nuclear physics) or smaller. If these levels are split by more than the pion mass, they can be detected by s-wave pion decay (or some other strong decay) of the higher state. If the mass difference is not so much, and the spin is $1/2$, then the dominant decay will involve the emission of photons via a pseudotensor coupling. However, these observations may not give the best signals for the detection of parity doublets. In fact, we can find none, comparable in elegance to the study of intensity alternation patterns in molecular physics alluded to previously, for the detection of such doublets in particle physics.

TABLE I. Constituent quark masses and their estimated lifetimes.

Quark	Constituent quark mass (GeV)	Constituent quark lifetime (sec)
u	~ 0.3	$\geq 10^{-6}$
d	~ 0.3	$\geq 10^{-6}$
s	~ 0.51	$10^{-6}-10^{-9}$
c	$1.1-1.6$	$10^{-11}-10^{-12}$
b	$4.1-4.5$	10^{-14}
t	170	10^{-22}

In the B-O approximation, the heavy quarks are not in a definite orbital angular momentum state, in contrast to what is found in quark models. For this and for other reasons, the relation of the B-O and quark model states is intricate and will be elaborated in [8].

Heavy mesons, Skyrmions, and monopoles.—Baryons are not the only favorable systems for parity doublets. Literature abounds in speculation [11,12] suggesting the existence of heavy meson bound states. They can involve distinct heavy mesons too. These can be the slow variables and suitable excitations (like the ρ or the ω meson) can be the fast ones, and we may have parity doublets again.

These doublets may also appear in the physics of Skyrmions and monopoles. For the former, there now exist elaborate simulations of static configurations for differing baryon numbers [13,14]. They are found to occur as regular solids with discrete symmetry groups.

TABLE II. T_{slow} and $T_{\text{slow}}/T_{\text{fast}}$ for baryons of interest.

Baryon	T_{slow} (sec)	$T_{\text{slow}}/T_{\text{fast}}$
scu/scd	$\sim 10^{-23}$	$2.9-3.5$
sbu/sbd	$\sim 10^{-23}$	$4.1-4.3$
stu/std	$\geq 10^{-22}$	4.5
cbu/cbd	$\sim 10^{-23}$	$8.8-11$
ctu/ctd	$\geq 10^{-22}$	$8.8-17.6$
btu/btd	$\geq 10^{-22}$	44

We can also imagine that further calculations will show static configurations such as a pear, with U(1) symmetry group. Excitations with spin, like a ρ or an ω, or even a nucleon, which can have nonzero helicity $\vec{n} \cdot \vec{J}_F$, could then lead to parity doublets.

Of equal interest to the above Skyrmion configurations are the static monopole configurations with symmetries under rotation subgroups [15–17]. They can occur in grand unified models. By attaching fast constituents such as a spin $1/2$ quark, we can hope to create parity doublets in these systems, just as in molecular physics.

A remark and a reminder.—Effects of heavy particle (slow core) spins are neglected in the B-O approximation. They could lead to additional degeneracies and may require future consideration.

It is crucial in these considerations that the slow configuration is reflection asymmetric for parity doublets to occur. They would not occur in *ccu*, as $c - c$ is described as a headless arrow. They would also not occur for staggered conformations which are reflection symmetric even though they can have a doublet structure mixed by $\mathcal{T}$. It would be most striking to encounter these $\mathcal{T}$ doublets, predicted naturally theoretically, in chemistry, and nuclear and particle physics.

Final remarks.—It is appropriate to conclude by outlining certain more formal considerations which we shall study elsewhere in greater depth [8].

The quantum theory of three-dimensional shapes, that is, quantization on configuration spaces $Q = \mathrm{SU}(2)/H$ was studied in [10]. As is well known [9,10], it is not unique, there being a distinct quantization for each unitary irreducible representation (UIR) ρ of H. For a particular ρ, the domain of the shape Hamiltonian $\mathcal{H}_S$ consists of sections of a vector bundle associated with ρ. These domains and hence the corresponding quantum theories are different for different ρ. Now, it so happens for reflection-asymmetric shapes that $\mathcal{P}$ can map ρ to an inequivalent UIR $\rho_{\mathcal{P}}$ and so the quantum theory to an inequivalent one. Quantum theory thereby spoils classical $\mathcal{P}$ invariance, in precisely the same manner that the presence of the topological θ term in QCD (for $\theta \neq 0, \pi$) breaks it [18,19]. Also $\rho_{\mathcal{P}} = \rho^*$ [10], so $\mathcal{T}$ is violated by quantization, but not $\mathcal{P}\mathcal{T}$. But the strange behavior of staggered conformations noted earlier is unlike anything we know of in conventional particle theory.

These results on shapes are paradoxical. There is no $\mathcal{P}$ or $\mathcal{T}$ violation in molecular physics while shapes (slow cores) with $\mathcal{P}$ or $\mathcal{T}$ violating ρ do occur in nature. How then is this paradox resolved?

The resolution is as follows. Let us at the start assume that the domain $V^{(\rho_0)}$ of the total Hamiltonian $\mathcal{H} = \mathcal{H}_S + \mathcal{H}_F$ is associated with the trivial representation ρ_0 that harms neither $\mathcal{P}$ nor $\mathcal{T}$. The domain of $\mathcal{H}_S$ is then also the domain associated with ρ_0. An eigenstate $\psi_F^{(\overline{\rho})}$ of the fast Hamiltonian $\mathcal{H}_F$ is the section of a vector bundle over Q in the B-O approximation (the Berry phase shows this result) [20,21] (the superscripts on wave functions will indicate the UIR), and it can happen that this bundle is twisted and is associated with a UIR $\overline{\rho}$. The B-O slow Hamiltonian is not $\mathcal{H}_S$, it must be obtained from averaging $\mathcal{H}$ over $\psi_F^{(\overline{\rho})}$, and when that is done, the emergent slow Hamiltonian $\hat{\mathcal{H}}_S$ contains a connection and has a domain associated with the UIR ρ, which is the complex conjugate of $\overline{\rho}$. (A result along these lines is in [20,21].) So an eigenstate $\psi_S^{(\rho)}$ of $\hat{\mathcal{H}}_S$ corresponds to ρ and the product wave function $\psi = \psi_S^{(\rho)}\psi_F^{(\overline{\rho})}$ corresponds to $\rho \otimes \overline{\rho}$. But $\mathcal{H}$ and $\mathcal{H}_S$ act on the total wave function and their domain can only correspond to ρ_0. That is now easily arranged as ρ_0 occurs in the reduction of $\rho \otimes \overline{\rho}$. The correct total wave function in the B-O approximation is thus the projection $\chi^{(\rho_0)} = \mathbf{P}[\psi_S^{(\rho)}\psi_F^{(\overline{\rho})}]$ of ψ to $V^{(\rho_0)}$. If $\rho_{\mathcal{P}} = \overline{\rho}$, the parity transform $\mathcal{P}\chi^{(\rho_0)}$ of $\chi^{(\rho_0)}$ is of the form $\mathbf{P}[\psi_S^{(\overline{\rho})}\psi_F^{(\rho)}] \in V^{(\rho_0)}$. It is still in the domain of $\mathcal{H}$ and $\mathcal{H}_S$, so there is no question of $\mathcal{P}$ violation. The same goes for $\mathcal{T}$. The doublets with definite $\mathcal{P}$ in the leading approximation are linear combinations of $\chi^{(\rho_0)}$ and $\mathcal{P}\chi^{(\rho_0)}$.

A remarkable feature of the B-O approximation, occasionally appreciated before, is that eigenstates of $\hat{\mathcal{H}}_S$ may be states with helicity [21], even spinorial states, even though those of $\mathcal{H}_S$ are tensorial zero-helicity ones. This happens if, for example, the configuration space Q is the two-dimensional sphere $S^2 = \{\vec{n}\}$. If the helicity $\vec{n} \cdot \vec{J}_F = -K$ of the $\mathcal{H}_F$ eigenstate is nonvanishing, then the slow wave function is a section of the monopole bundle with helicity (Chern number) K. The slow wave function is then spinoral if $K \in (2Z + 1)/2$. A spinorial slow eigenfunction can get converted to a tensorial one too under suitable conditions.

Now suppose that the fast variables (with UIR $\overline{\rho}$) cannot be seen by current experiments, perhaps because their excitations are too energetic. They can still leave a trace in the slow system by twisting its bundle from ρ_0 to ρ or changing its prior twist, and perhaps even altering its tensorial or spinorial character. If, without our being aware, the fast variable for UIR $\overline{\rho}$ is replaced by another for UIR ρ', the slow bundle is thereby also changed. This is an effective topology change, but at a quantum level, for the Hamiltonian $\mathcal{H}_S$. The topology change of classical configuration space, frantically sought in gravity, cannot be achieved in this manner. That would require another mechanism like cobordism in functional integrals [22] or domain changes (of a new sort) of the Hamiltonian [23].

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