PHASE TRANSITIONS IN QCD AS TUNNELING THROUGH SINGULAR BARRIERS

C.G. CALLAN [1]
Princeton University, Princeton, NJ 08540, USA

R. DASHEN [2] and D. GROSS [3]
Institute for Advanced Study, Princeton, NJ 08540, USA

Received 10 May 1978

We show that the phase transitions of QCD, chiral symmetry breaking and confinement, can be interpreted physically as tunneling through (infrared) singular barriers. The appearance of monopoles in QCD and the properties of massless fermions in a meron field are discussed in the context of this interpretation.

Between perturbation theoretic QCD and real hadrons lie two phase transitions, confinement and chiral symmetry breaking. In this paper we give a simple interpretation of these phase transitions in terms of tunneling through singular barriers. The observation that the BPST instanton [1] represented quantum mechanical tunneling [2] between classical vacua was useful in that it gave the instanton a home in the usual conceptual framework of quantum mechanics. Our purpose here is to do the same thing for some more complex phenomena. One must remember however that a simple tunneling picture has problems in field theory. In QCD tunnelings are localized in space as well as time and it is difficult to say whether or not a specific tunneling transition has actually taken place, since it might have been accompanied by a distant anti-tunneling. A framework which avoids this difficulty is the analog gas picture [3] where the tunnelings are thought of as (pseudo-)particles in a four dimensional gas. We will need only one concept from this gas picture, the entropy of a configuration. It is the log of the volume in function space occupied by similar configurations and is usually computed by doing a gaussian functional integral about the basic configuration. For a single localizable tunneling which can occur anywhere in a box of volume V or at any time in an interval of length T the entropy contains a term $\ln(VT)$.

To see how singular barriers arise, recall that in a ϕ^4 theory, $\mathcal{L} = \frac{1}{2}(\partial_\mu\phi)^2 - \lambda(\phi^2 - F^2)^2$, there is no tunneling between the vacua $\phi = \pm F$. The reason is, of course, that in an infinite volume any path connecting $\phi = F$ to $\phi = -F$ has infinite action, i.e. the barrier between F and $-F$ is singular. In quantum mechanics singular barriers can arise only from actual singularities in the potential. In field theory, on the other hand, they generally come about because the tunneling time history has an action integral $\int d^4x\,\mathcal{L}$ which diverges at infinity, i.e. the singularity is an *infrared* one. In what follows we will see that barriers with a mild infrared singularity, $S = \frac{1}{4}J\log(VT)$, are sometimes penetrable and that the subsequent tunneling leads to a phase transition. To see why such a barrier might be penetrated we note that it is not only the action but also the entropy that counts [4,5]. If a tunneling has a point of localization we expect a tunneling amplitude $VTe^{-S} = \exp[-S + \log(VT)]$ and if $S = \frac{1}{4}J\log(VT)$ with $J < 4$ the complete amplitude does not vanish as $VT \to \infty$. Logarithmic infrared singularities like $S \propto \log(VT)$ are typical of scale invariant theories such as QCD and do in fact occur here.

[1] Research supported in part by National Science Foundation Grant No. PHY 78-01221.
[2] Research supported in part by Department of Energy Grant No. EY-76-S-02-2220.
[3] On leave from Princeton University. Research supported in part by National Science Foundation Grant No. PHY 77-20612.

There is an amusing (but, we warn, in some ways misleading) example of singular barrier penetration in ordinary quantum mechanics. For a particle on a line $-\infty < x < \infty$ the (imaginary time) action $S = (1/g^2) \times \int [\frac{1}{2}\dot{x}^2 + x^{-2}]\, dt$ defines a scale invariant theory with a non-linear coupling constant defined according to the usual field theoretic convention. Let us make a simple estimate of when the repulsive x^{-2} barrier can be penetrated. Away from $t = 0$ the euclidean equations of motion have a solution $x = \pm(8t^2)^{1/4}$ for $t \gtrless 0$. We will assume that the potential and/or tunneling path has somehow been regulated at $x = t = 0$ [6]. Then, putting the system in a time box, the euclidean action will diverge like $(\sqrt{2}/g^2) \log T$. Since the barrier is penetrated at a definite time we expect an entropy $\log T$ and tunneling for $g^2 > \sqrt{2}$. This calculation is not very accurate for a number of reasons. First we really should regulate the model and compute the gaussian integral around a regulated tunneling path: one would expect the fluctuations to add a term O(1) [$\log T$] which in field theory would be interpreted as a coupling renormalization. Also as we will see below the criterion action = entropy is precise only for weak coupling. Fortunately we do not have to go through a long calculation of determinants etc., because the model is trivially soluble quantum mechanically. The Schrödinger equation $[-\frac{1}{2}d^2/dx^2 + 1/g^4x^2]\,\psi = k^2\psi$ has (Bessel function) solutions $\sqrt{x}\, J_{\pm\alpha}(kx)$ where $\alpha^2 = (2/g^4 + \frac{1}{4})$. For $g^2 < (8/3)^{1/2}$, $\sqrt{x}\, J_{-\alpha}(kx)$ is not square integrable at the origin and the only allowed solutions are the $\sqrt{x}\, J_{+\alpha}$'s. All wave functions then vanish at $x = 0$ and the regions $x > 0$ and $x < 0$ are separate worlds which do not communicate. However, for a coupling $g^2 > (8/3)^{1/2}$, $\sqrt{x}\, J_{-\alpha}$ is square integrable at the origin and we have to decide whether or not to keep the singular but square integrable eigenfunctions. Purely within quantum mechanics there is no definite answer to this question (technically the formal hamiltonian has more than one self adjoint extension [6]). In field theory, on the other hand, the instruction would be to put the system in a box and choose that "phase" for which the ground state energy is the lowest. It is easy to verify that in a box the lowest energy state is $\sqrt{x} J_{-\alpha}$ and we conclude that in an analogous field theory there would be tunneling (the wave functions no longer vanish at $x = 0$) for $g^2 > (8/3)^{1/2}$, not far from our simple estimate $g^2 > (2)^{1/2}$. The essentials of this "phase transition" are a scale invariant singular barrier and a sufficiently large coupling. These will carry over to field theory but because a tunneling trajectory has to pass through $x = 0$, producing a singularity in the action which is not purely infrared, the model can be otherwise misleading. In fact, the major defect of the above model is that it does not allow virtual penetration of the barrier before the phase transition. In a conformally invariant field theory such as QCD, the appearance of (localizable) infrared singular tunneling can always be thought of as an "ionization" process; i.e. the separation of a tunneling and anti-tunneling. To see this, consider a localizable tunneling with a core of size ρ in a space–time box of radius $R = (VT)^{1/4} \gg \rho$ and with an action $J \ln(R/\rho)$. If the tunneling is located at the origin, an inversion

$$(x - \sqrt{R\rho}\, n)^\mu \rightarrow (x - \sqrt{R\rho}\, n)^\mu\, R\rho/(x - \sqrt{R\rho}\, n)^2$$

(with $n^2 = 1$) produces a configuration where the box is mapped into a sphere of radius ρ centered at the origin and the core of the tunneling remains of size ρ but is now located at $\Delta^\mu = \sqrt{R\rho}\, n^\mu$ (fig. 1). The inverted configuration has fields that are well behaved at infinity and a finite action $2J\ln(|\Delta|/\rho)$. The image of the box can be interpreted as an anti-tunneling and the configuration describes a correlated tunneling and anti-tunneling held together by an (apparently) confining

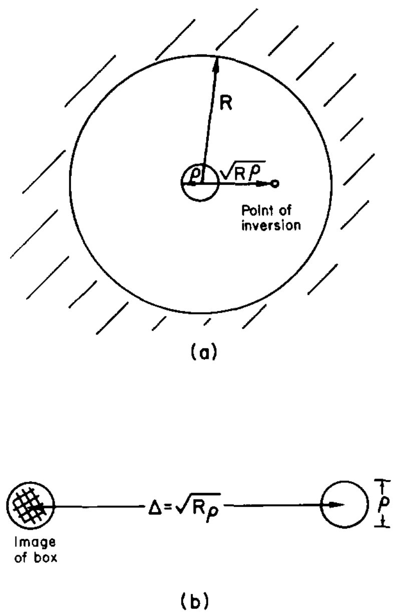

Fig. 1. The inversion which takes a tunneling in a box (a) to a tunneling–anti-tunneling pair (b) separated by $\Delta = \sqrt{R\rho}$.

logarithmic potential. The picture of the phase transition is then as follows. If J is so large that the barrier cannot be penetrated tunnelings and anti-tunnelings are permanently bound together into "diatomic molecules". In this molecular phase the singular tunneling is virtual and exists only over the space–time volume of the molecule. When J decreases to the point where the singular barrier can be penetrated, this complete pairwise correlation is replaced by a less restrictive one, e.g. Debye correlations (fig. 2).

The notion of a phase transition in systems with logarithmic actions, can be made precise by an observation of Kosterlitz and Thouless [4]. Suppose that in d dimensions the density of some objects of size ρ in a box of radius R is $\xi\rho^{-d}\exp[-J\ln(R/\rho)]$ or equivalently (by an inversion) the density of virtual pairs separated by Δ is $\xi^2\rho^{-2d}\exp[-2J\ln(\Delta/\rho)]$, where ξ and J are pure numbers. The parameter ξ is a kind of dimensionless density; taking ξ to zero produces an arbitrarily dilute system. In applications to QCD ξ and J cannot necessarily be varied independently (if at all) but it is instructive to consider what would happen if they could be. The result of Kosterlitz and Thouless is that in the limit $\xi \to 0$ there is a critical point at $J = d$ (just the place where action equals entropy) and that for ξ infinitesimally above zero the critical point is at $J > d$. Thus the first-order effect of finite density is to increase the critical J. The phase diagram is shown in fig. 3. The behavior for finite ξ is uncertain but on physical grounds one expects the critical point to move to larger J as ξ increases.

In practice one does not always have the luxury of

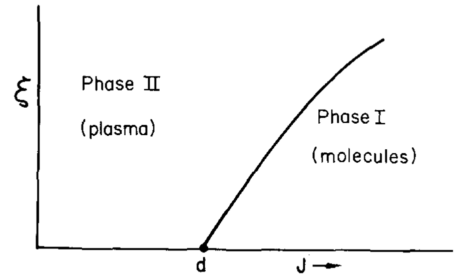

Fig. 3. The Kosterlitz–Thouless phase diagram.

looking near $\xi = 0$. The reason can be seen already in the quantum mechanical model. There $J = \sqrt{2}/g^2$ and ξ, which must be $\sim e^{-1/g^2}$, are not independent. Thus the phase transition which can only occur at a finite g and hence finite ξ cannot be precisely located by the Kosterlitz–Thouless arguments. However, the general picture would strongly suggest that the phase transition occurs at a g^2 less than $\sqrt{2}$, as indeed it does. We will now proceed to apply these ideas to QCD.

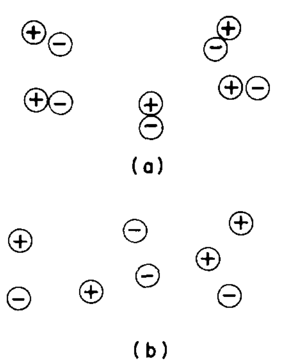

Fig. 2. Tunneling–anti-tunneling pairs in a molecular phase where singular barrier penetration is virtual. (b) The plasma phase after the barrier is penetrated.

It is well known that massless fermions supress vacuum tunneling [2,3]. Formally, the Dirac operator $\not{D}$ has a (normalizable) eigenvector with an eigenvalue that vanishes like $R^{-(d-1)}$ in a large box. Physically the tunneling is vac $\to \bar{q}_L q_R$ rather than vac $\to$ vac and is supressed because the quarks must go into exactly zero energy states, spreading out the fields to the point that the barrier becomes divergent. Equivalently, instanton–anti-instanton pairs are bound together by massless fermion exchange. This produces an effective potential $2(d-1)N_f \ln\Delta$, where N_f is the number of massless flavors. When the singular barrier can be penetrated it is quite clear that chiral symmetry will be broken [5,7,8]. The tunneling process vac $\to$ vac $+\ \bar{q}_L q_R$ will make the physical vacuum a coherent superposition of states containing many $\bar{q}_L q_R$ pairs and there will be a non-zero expectation value of $\bar{q}q$. For massless fermions the Kosterlitz–Thouless point at $\xi = 0$ is $N_f = d/(d-1)$. In two dimensions there is a model [8] in which ξ can be made as small as one likes and explicit calculations show that $N_f = 2$ is the critical point. In four dimensions the Kosterlitz–Thouless point is $N_f = 4/3$ and a phase transition is automatic for $N_f = 1$ but requires finite density for $N_f \geqslant 2$. This is in agreement with ref. [3] where it is also shown that in QCD the density of instantons is in fact sufficient to produce a phase transition for $N_f \geqslant 2$.

Confinement can also be attained by the penetration of a singular barrier [5]. This time the object which ionizes is the instanton itself. The meron, $A_a^\mu = \eta_a^{\mu\nu} x^\nu/x^2$, satisfies the euclidean Yang–Mills equations [9] and has one half unit of topological charge, $(1/8\pi^2)\int \mathrm{tr}\, F\tilde{F}\, \mathrm{d}^4x$, located at the origin. Topologically the meron is half an instanton. In asymptotically free QCD the singularity at the origin can be freely smeared out over an arbitrarily chosen distance ρ and the action of a meron in a box is then $S = (3\pi^2/g^2) \times \ln(R/\rho)$. The entropy of a meron is then well defined [3] and the Kosterlitz–Thouless point for zero density turns out to be $\bar{g}^2/8\pi^2 = 3/32$, where $\bar{g}$ is a running coupling defined in ref. [3]. Because the density of meron pairs is finite the transition will actually be at $\bar{g}^2/8\pi^2 < 3/32$, a remarkably small coupling. That the phase transition actually leads to confinement is strongly suggested by showing that at the transition the static coupling constant begins to diverge [3].

To see the nature of the singular tunneling represented by merons it is useful to pass to the gauge $A^0 = 0$, where

$$A_a^k(x, t) = \epsilon_{akj} \frac{x^j}{|x|^2} \left(1 + \frac{t}{\sqrt{x^2 + t^2}}\right).$$

For $t = -\infty$, A vanishes while for $t \to +\infty$, it is a pure gauge $\mathrm{i}A = S^{-1}\nabla S$ with $S = \exp[\mathrm{i}\pi\tau\cdot\hat{x}/2] = \mathrm{i}\tau\cdot\hat{x}$ corresponding to a (transverse) vacuum field with winding number one half. At the time when the barrier is penetrated ($t = 0$) the fields form a Wu–Yang monopole $\epsilon_{akj}x_j/x^2$. There is a reason why the monopole is there. In a potential theory model $L = \frac{1}{2}\dot{x}^2 + \lambda(x^2 - 1)^2$ the instanton connects two vacua, $x = \pm 1$, related to each other by the symmetry operation P: $x \to -x$. A tunneling trajectory crosses the top of the barrier at a point $x = 0$ which is invariant under P. The meron connects states related to each other by the gauge transformation S. It crosses the top of the barrier at a monopole field configuration $\mathrm{i}A = \frac{1}{2}S^{-1}\nabla S$, which is invariant under S. When this singular barrier is penetrated at $g^2/8\pi \approx 3/32$ the wave function of the vacuum will be nonzero at the monopole configuration, leading to a connection with Mandelstam's [10] ideas of confinement via monopoles in the vacuum.

We have assumed here that the order of the phase transitions is chiral symmetry breaking followed by confinement. It is possible that they both occur at the same time in which case the picture would be one of bound instanton–anti-instanton pairs dissociating directly into meron–anti-meron pairs. What actually happens is a quantitative question and calculations suggest the two step process [3]. However, it is amusing to speculate about how a single step process would look. In $A^0 = 0$ gauge and thinking about imaginary time t as a parameter the eigenvalues $\epsilon_i(t)$ of the static Dirac operator $\boldsymbol{\alpha}\cdot \boldsymbol{D}(t)\psi_i = \epsilon_i(t)\psi_i$ in an instanton field have the property that $\epsilon_i(+\infty) = \epsilon_{i-1}(-\infty)$ for the right handed states and $\epsilon_i(+\infty) = \epsilon_{i+1}(-\infty)$ for the left handed states (the index i orders the discrete, finite space box, eigenvalues according to energy from $-\infty$ to $+\infty$). Thus in the tunneling process the spectrum of $\boldsymbol{\alpha}\cdot\boldsymbol{D}$ is mapped into itself with one right handed state crossing zero from below and a left handed state crossing zero from above. A hole theory argument then shows why the tunneling is vac $\to \bar{q}_L q_R$. In a meron field, however, one of the eigenvalues $\epsilon(+\infty)$ is identically zero. In hole theory a zero eigenvalue for the three dimensional Dirac equation causes trouble: one does not know whether this state is a fermion or an anti-fermion. Thus it may be difficult to define strictly massless colored fermions in the presence of free merons. This is probably why merons confine in the Schwinger model [11]. In terms of the four dimensional Dirac equation the fermion zero mode in the field of an instanton located at x_0 gives, for large $|x_i - x_0|$,

$$\langle \bar{\psi}_L(x_1)\psi_R(x_2)\rangle \sim (x_1 - x_0)^{-3}(x_2 - x_0)^{-3},$$

corresponding to pair production at the instanton. A pair of merons located at x_1 and x_2 also have a zero mode which implies that

$$\langle \bar{\psi}_L(x)\psi_R(y)\rangle \sim (x - x_1)^{-3/2}(x - x_2)^{-3/2} \times (y - x_1)^{-3/2}(y - x_2)^{-3/2}.$$

This has the appearance of a square root (!) of a fermion propagator ending at each meron. It is as if each meron is equivalent to an insertion of "$\sqrt{\bar{\psi}_L\psi_R}$"!

One might even speculate that if singular tunneling exists in QCD then one could define local operators which act like $\sqrt{\bar{\psi}\psi}$. This is because in the presence of singular tunneling the Hilbert space would be enlarged, containing sectors with both integer and half-integer winding number gauge fields. Since a winding number zero sector and a winding number one-half sector differ in their axial baryon number by N_f (where N_f is the number of massless fermions) and since the singular tunneling is achieved via localizable meron configurations there should exist localizable operators which act like $(\det_{i,j}\bar{\psi}_{iR}\psi_{jL})^{1/2}$ (where $i, j = 1, \dots, N_f$). We do not know how to explicitly construct such operators.

Finally we note the relation between our discussion of tunneling through a singular barrier and the choice of boundary conditions in the euclidean path integral. One normally requires $r^2F_{\mu\nu}(r) \to 0$ as $r_\mu = \to \infty$ so as to yield finite action time histories. These strong boundary conditions then exclude single meron configurations and tunneling events that change the winding number by one half. However the correct choice of boundary conditions is a dynamical issue that can only be resolved by calculation. According to our discussion above, isolated meron configurations might very well contribute to the path integral for sufficiently strong coupling, thus forcing one to relax the strong boundary condition and allow for fields (i.e. meron fields for which $r^2F_{\mu\nu} \to$ const as $r \to \infty$). This is analogous to the relaxation of the Dirichlet boundary conditions imposed on the singular potential $V = 1/g^4x^2$ for $g^2 > \sqrt{8/3}$.

Once one is forced to relax the condition of strong boundary conditions and allow for isolated meron path histories the quantization of non-abelian gauge theories becomes problematic. In particular one is then forced to consider the problems raised by Gribov [12] who has shown the vacuum state in Coulomb gauge is non-unique. In fact the meron time history interpolates between an $A_\mu = 0$ configuration (in $A_0 = 0$ gauge) at $t = -\infty$ and Gribov's transverse gauge field $A_i^a = 2\epsilon_{aij}x_j/x^2$ at $t = +\infty$.

In conclusion, we have shown how the phase transitions of QCD can be interpreted as tunneling through infrared singular barriers. This makes the physical interpretation clear but we do not advocate a tunneling formalism for actual calculations in QCD. In practice it turns out to be much easier to discuss the euclidean functional integral and to deal with the analog gas picture, which has led to a number of fruitful analogies between QCD and paramagnetism and to a model of confined quarks [13].

References

[1] A. Belavin, A. Polyakov, A. Schwartz and Y. Tyupkin, Phys. Lett. 59B (1975) 85.
[2] G. 't Hooft, Phys. Rev. Lett. 37 (1976) 8;
C. Callan, R. Dashen and D. Gross, Phys. Lett. 63B (1976) 334;
R. Jackiw and C. Rebbi, Phys. Rev. Lett. 37 (1976) 172.
[3] C. Callan, R. Dashen and D. Gross, IAS preprint COO-2220-115, to be published in Phys. Rev. D.
[4] J. Kosterlitz and D. Thouless, J. Phys. C6 (1973) 1181.
[5] C. Callan, R. Dashen and D. Gross, Phys. Lett. 65B (1977) 375.
[6] J.R. Klauder, Acta Phys. Austr. Suppl. X1 (1973) 341; Phys. Lett. 47B (1973) 523.
[7] D. Caldi, Phys. Rev. Lett. 39 (1977) 121.
[8] C. Callan, R. Dashen and D. Gross, Phys. Rev. D16 (1977) 2526.
[9] V. de Alfaro, S. Fubini and G. Furlan, Phys. Lett. 65B (1977) 1631.
[10] S. Mandelstam, Phys. Rep. 23 (1975) 245.
[11] N. Nielson and B. Schroer, Phys. Lett. 66B (1977) 475.
[12] V. Gribov, Leningrad preprint 1977, to be published in Nucl. Phys.
[13] C. Callan, R. Dashen and D. Gross, A theory of quark confinement, IAS preprint.