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SUM OVER CONFIGURATIONS

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The first article in Ref. 2) should be :

R. Finkelstein, R. LeLevier and M. Ruderman, Phys.Rev. 83, 326 (1951)

rather than

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I wish to apologize to R. Finkelstein, R. LeLevier and
M. Ruderman for having omitted their reference in previous publi-
cations.

"SUM OVER CONFIGURATIONS"
(NON-PERTURBATIVE QUANTUM EXPANSION FOR SOLITONS
AND OTHER STATES IN FIELD THEORY)

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A B S T R A C T

Models of hadrons and temporary quark confinement, based on field theories with extended classical solutions, neglect quantum fluctuation effects. To account for these effects, we propose systematic expansions for the vacuum, one-particle and collision states which are non-perturbative. Their order is not a power of any coupling constant, but a number of field configurations. To exhibit the conceptual and technical simplicity of the method, we study fluctuations describing virtual soliton-antisoliton pairs in a model theory. We also propose a "hybrid approximation" for non-perturbative calculations of scattering amplitudes.

If hadrons are described by a quantum field theory (which is the author's prejudice), field theories with extended classical solutions¹⁻⁴⁾ start off as particularly strong candidates. The quantization of these theories has been approached so far in one of two ways: a) by a non-perturbative variational method^{1,4,5)}; b) in perturbation theory^{6,7)}. Perturbative approaches are systematic, but presumably inapplicable to the actual physical problem which involves strong couplings. The variational method described in Refs. 1, 4 and 5 is, on the other hand, suited to a strong coupling régime but lacks systematics: it is based on guesses and does not define procedures for improving the approximations.

This difficulty can be remedied. In this note, we shall in fact propose systematic non-perturbative variational expansions for the vacuum^{*)}, one-particle and collision states which provide well-defined procedures for improving the approximations for such states to an arbitrarily high degree. The approach will be conceptually transparent and technically relatively simple.

To introduce our proposal and clarify its relevance, it will perhaps be helpful to consider first the following kindergarten problem in ordinary one-particle quantum mechanics. Suppose we had to determine the quantum ground state of an anharmonic oscillator with the potential represented by Fig. 1. The classical ground state of this system is the configuration defined by the coordinate $q = 0$ and momentum $p = 0$. Classically there also exists a stable stationary configuration corresponding to the secondary minimum, $q = -\lambda$ and $p = 0$. Quantum-mechanically these configurations are expected to be connected by "tunnelling" and should both contribute to the ground state. In order to describe the quantized system, we construct a harmonic oscillator Fock space around the classical ground-state configuration. Thus we define a vacuum state, $|0\rangle$, annihilated by the operator $(1/\sqrt{2})(q + ip)$,

$$\frac{1}{\sqrt{2}} (q + ip) |0\rangle = 0,$$

whose configuration space representation is, of course, a Gaussian centred at $q = 0$. This state provides the standard zeroth order approximation to the true ground state, $|\Omega\rangle$, of the system.

To improve this approximation we may now want to proceed in perturbation theory. We would then easily discover (relatively unimportant) correction terms due to the anharmonicity of the potential around $q = 0$. But, in finite orders, we would never discover the (major) contribution due to the secondary minimum of the potential at $q = -\lambda$.

*) Thus, our method can also be applied to investigate the occurrence of ("dynamical") spontaneous symmetry breakdown due to quantum effects, in absence of ("ad hoc") driving terms in the classical potential and of spinless fields.

Alternatively, we may want to expand the true ground state as follows

$$|\Omega\rangle = \alpha|0\rangle + \beta e^{-i\xi\phi}|0\rangle + \dots$$

and determine the *a priori* arbitrary c-numbers α , β , and ξ by a variational calculation. We would then immediately discover effects of the secondary minimum at $q = -\lambda$ and our "first-order" approximation to $|\Omega\rangle$,

$$\langle q|\Omega\rangle \simeq \alpha e^{-\frac{1}{2}q^2} + \beta e^{-\frac{1}{2}(q+\lambda)^2},$$

would be a great improvement over the zeroth-order one.

Turning to field theory, an analogous situation presents itself if Fig. 1 is now thought of as representing the self-interaction potential of (say) a scalar field ϕ , as in popular quark-confinement models^{1,4}). Although (because of lack of tunnelling in a system with infinitely many degrees of freedom) the configuration $\phi = -\lambda$, $\dot{\phi} = 0$ would itself not play any role in determining the true ground state of the system, other configurations corresponding to "localized excitations of the secondary potential minimum"¹⁾ would indeed play an important role. And, again, these configurations would not be accessible in perturbation theory.

To cope with the presence of such global field fluctuations, involving infinite numbers of quanta and generally important in theories with strong couplings (even in the absence of secondary minima of field potentials), we shall therefore abstract a strategy suggested by the previous example: following procedures to be specified in a moment, we will non-perturbatively expand states in "sums over field configurations". This approach is based on a physical picture of the connection between quantum and classical fields that is inspired by Feynman's "sum over histories" prescription for Green's functions⁸⁾. Notice, however, that our approach applies to states in Hilbert space which in the Heisenberg representation, in which we work, are time-independent and, hence, have no history.

To become more specific, let us consider the theory of a real scalar field ϕ in one-space-one-time dimension with the Hamiltonian density^{*)}

$$\mathcal{H} = : \frac{1}{2} \pi^2 + \frac{1}{2} \phi'^2 + \frac{1}{4} (\phi^2 - \lambda^2)^2 : \quad (1)$$

Here, $\pi(x)$ is the momentum conjugate to the field $\phi(x)$, an expansion of π and ϕ at time $t = 0$ into plane waves and the associated choice of a base in Fock space has been implied, and the colons denote normal ordering in such a base. We shall

*) This model has been recently discussed by a number of authors. See, for example, Refs. 5 and 6.

represent Fock space states $|s\rangle$ by double functional integrals

$$|s\rangle = \frac{1}{S} \iint \mathcal{D}f \mathcal{D}g \mathcal{F}(f, g) |f, g\rangle \quad (2)$$

in terms of coherent states⁹⁾

$$|f, g\rangle = \exp[-i\pi(f) + i\phi(g)] |0\rangle. \quad (3)$$

Here, S is a normalization factor, $|0\rangle$ denotes the Fock space no-particle state and $\phi(g)$ $[\pi(f)]$ denotes the field $\phi(x)$ $[\pi(x)]$ smeared with the real function $g(x)$ $[f(x)]$ of the space coordinate x . Since

$$\langle f, g | : \tilde{\phi}(x) : | f, g \rangle = \tilde{f}(x), \quad \langle f, g | : \tilde{\pi}(x) : | f, g \rangle = \tilde{g}(x), \quad (4)$$

$f(x)$ and $g(x)$ define configurations of the classical field^{*)} and the representation (2) is an infinite "sum over configurations"^{**) .}

The eigenstates corresponding to the lowest or highest eigenvalue of some operator $\mathcal{O}$ ("extremal states of $\mathcal{O}$ ") may be constructed in the representation (2) by solving the variational equations

$$\frac{\delta}{\delta \mathcal{F}(f, g)} \langle s | \mathcal{O} | s \rangle = 0. \quad (5)$$

Thus, in particular, if $\mathcal{O}$ is identified with the Hamiltonian corresponding to the density (1), $\mathcal{O} \equiv \mathcal{H} = \int dx \mathcal{H}(x)$, the solutions to these equations in the vacuum sectors

$$f(x) \begin{cases} \rightarrow \pm \lambda, & x \rightarrow +\infty \\ \rightarrow \pm \lambda, & x \rightarrow -\infty \end{cases} \quad (6)$$

will yield the functional $\mathcal{F}(f, g)$ corresponding to the vacuum states $|\Omega_{\pm}\rangle$; and the solutions to the same equations in the one-particle ("soliton") sectors

*) Configurations of scalar fields, for which the equations of motion are of second order, are of course specified by knowledge of the field and its time derivative on a space-like surface.

**) Note that expansions analogous to (2) exist also for vector and (with the help of anti-commuting c-numbers) spinor fields,

$$f(x) \begin{cases} \rightarrow \pm \lambda, & x \rightarrow +\infty \\ \rightarrow \mp \lambda, & x \rightarrow -\infty \end{cases} \quad (7)$$

will yield the functional $\mathcal{F}(f,g)$ corresponding to the zero-momentum "soliton" states, $|p=0\rangle$.

However, as they stand, the representation (2) and Eqs. (5) are manifestly too complicated to be useful. Since we are, in any case, seldom interested in an exact characterization of a state, we therefore propose to (approximately) replace (2) with a finite sum over configurations:

$$|S\rangle_N = \frac{1}{S_N} \sum_n^N a_n |f_n, g_n\rangle. \quad (8)$$

Notice that, if this approximation is to preserve Poincaré invariance, the finite summation can never be intended in a strict sense, but must include integrals over configurations related by boosts, rotations, and translations. If we think of these as forming an equivalence class, the expression (8) should therefore be intended as a finite sum over equivalence classes.

Once we have accepted the ansatz (8), the problem at hand becomes the determination of "the N most relevant configurations" (f_n, g_n) in the description of a state $|S\rangle$ and of the associated coefficient amplitudes a_n . For extremal states of some operator $\mathcal{O}$, we are now led to a finite system of coupled integro-differential equations

$$\frac{\delta}{\delta f_n(x)} \langle S | \mathcal{O} | S \rangle_N = \frac{\delta}{\delta g_n(x)} \langle S | \mathcal{O} | S \rangle_N = 0 \quad (9')$$

and algebraic equations

$$\frac{d}{da_n} \langle S | \mathcal{O} | S \rangle_N = 0. \quad (9'')$$

Although simpler than (5), it is clear that, in general, for large N this system will put too much strain on one's technical abilities.

Fortunately, at the expense of some compromise in the rapidity of convergence of the expansion (8), further dramatic technical simplifications in the description of such states may be achieved. Three different methods immediately come to mind. They are, in order of increasing technical simplicity:

i) Iterative procedure

An N^{th} order approximation is constructed from the $(N - 1)^{\text{th}}$ by

$$|s\rangle_N = \frac{1}{N_N} (\alpha_N |s\rangle_{N-1} + \beta_N |f_N, g_N\rangle). \quad (10)$$

The functions defining the N^{th} configuration (f_N, g_N) and the coefficient amplitudes (α_N, β_N) are determined as solutions of variational equations involving previously obtained configurations as fixed external functions. Apart from the appearance of a different number of external functions, the equations to be solved in different orders have the same structure. The sequence $|s\rangle_N$ so constructed converges less fast than the sequence obtained by solving systems such as (9). This may be a small price to pay for the considerable degree of technical simplification that has been gained.

ii) Expansion in classical configurations

Suppose that the classical dynamics of the system under consideration is known (at least in part or approximately), i.e. that (static and time-dependent) solutions to the classical field equations satisfying appropriate boundary conditions are known. Since the functional $\mathcal{F}_s(f, g)$ in Eq. (2) is expected to peak around classical configurations, these solutions^{*} provide a natural basis for the expansion (8). Notice, in particular, that configurations which belong to the same periodic time-dependent solution $[f(t), g(t)]$ have a natural relative weight induced by the solution itself via the orbital integral

$$\int_0^T dt |f(t), g(t)\rangle \quad (11)$$

over an internal time-parameter t . This classical weight may be adopted by including directly states such as (11) in the expansion (8). With the configurations (f_n, g_n) in Eq. (8) *a priori* determined, variational equations now reduce to a trivial system of algebraic equations for the unknown coefficient amplitudes in Eq. (8). In a different language, a representation of the operator $\mathcal{O}$ in the subspace spanned by the states $|f_n, g_n\rangle$ which are

^{*}) Taken, e.g., in order of increasing energy.

not orthogonal to each other, $\langle f_i, g_i | f_j, g_j \rangle \neq 0$, is known in terms of the matrix elements

$$\langle f_i, g_i | \mathcal{O} | f_j, g_j \rangle = \mathcal{O}_{ij} . \quad (12)$$

The determination of extremal states of $\mathcal{O}$ within that subspace is, of course, as trivial as diagonalizing a finite-dimensional matrix.

iii) Random expansions

Lacking knowledge of solutions to the classical equations for the true Hamiltonian $\mathcal{H}$, one may use knowledge of the eigenfunctions of a Hamiltonian "similar" to $\mathcal{H}$ to provide configurations for the expansion (8), and then proceed to solve a simple algebraic problem as above. How far these approaches can be carried out by numerical techniques is clearly only limited by one's patience... and the computer time at one's disposal!

To show our approach at work, we shall now describe some model calculations^{*)}. These calculations are very simple. Yet they provide interesting physical insight.

In lowest order, our expansion over field configurations involves only one configuration. The variational equations (9'), with the operator $\mathcal{O}$ identified with the Hamiltonian $\mathcal{H}$ corresponding to the density (1), reduce to the condition $g(x) = 0$ and the time-independent classical field equation for $f(x)$. The solutions (configurations)

$$g_i(x) = 0 , \quad f_i(x) = \pm \lambda \quad (13')$$

$$g_i(x) = 0 , \quad f_i(x) = \pm f_s(x) = \pm \lambda \tanh(\lambda \sqrt{2H} x) \quad (13'')$$

yield the lowest order approximations to the vacua and one-particle "soliton" states. Notice that while this approximation to the vacua is Poincaré invariant, this approximation to soliton states is not. However, as the requirement of Poincaré invariance is a technical problem which needlessly complicates some of the issues, we shall ignore it for the moment.

In the spirit of the program outlined above, we now would like to improve on the approximation (13) by taking into account the effect of configurations corresponding to soliton-anti-soliton pairs at rest, both in the vacuum and soliton sectors:

*) Analogous calculations may be carried out to account for quantum fluctuation effects in more realistic models such as that of Ref. 1.

$$g_2(x) = 0, \quad f_2(x) = \pm \lambda \mp f_s(x+x_0) \pm f_s(x-x_0) \quad (14')$$

$$g_2(x) = 0, \quad f_2(x) = \pm f_s(x) \mp f_s(x+x_0) \pm f_s(x-x_0). \quad (14'')$$

The separation of the pair, $2x_0$, is taken as a free parameter. Again, we simply identify $\mathcal{O}$ with the Hamiltonian $\mathcal{H}$. We then have to minimize its expectation value within the trial states:

$$|S\rangle = \frac{1}{\sqrt{S}} (\alpha |f_1\rangle + \beta |f_2\rangle). \quad (15)$$

Off-diagonal matrix elements (of the Hamiltonian density) between two different coherent states are calculated from the identity

$$\langle f_1 | : \phi^n(x) : | f_2 \rangle = \left[\frac{f_1(x) + f_2(x)}{2} \right]^n e^{-\frac{1}{2} \|f_1 - f_2\|^2} \quad (16)$$

where

$$\|f\|^2 = \langle \pi(f)^2 \rangle = \frac{1}{2} \int dp (m_0^2 + p^2)^{1/2} |\tilde{f}(p)|^2. \quad (17)$$

In Eq. (17), m_0 is to be identified with the classical meson mass, $m_0 = 2\sqrt{2H} \lambda$, and $\tilde{f}(p) = 1/\sqrt{2\pi} \int dx e^{ipx} f(x)$. Taking $x_0 > 1/m_0$, we find for the Hamiltonian expectation value within states (15), corresponding to the vacuum and soliton sectors, respectively:

$$\langle S | \mathcal{H} | S \rangle_{vac} \approx \mu_0 \left\{ 2\beta^2 + \frac{3}{4} \alpha \beta m_0 x_0 e^{-3\mu_0 x_0} \right\} / S \quad (18')$$

$$\langle S | \mathcal{H} | S \rangle_{sol} \approx \mu_0 \left\{ \alpha^2 + 3\beta^2 + \frac{3}{4} \alpha \beta m_0 x_0 e^{-3\mu_0 x_0} \right\} / S \quad (18'')$$

$$S \approx \alpha^2 + \beta^2 + 2\alpha\beta e^{-3\mu_0 x_0} \quad (19)$$

where μ_0 denotes the classical soliton mass, $\mu_0 = \frac{4}{3} \sqrt{2H} \lambda^3$. Minimization of expressions (18') and (18''), with respect to the coefficient amplitudes α and β defined by Eq. (15), yields the vacuum and soliton energies:

$$E_{vac} = \mu_0 \xi_{vac} \left(\frac{m_0}{\mu_0}, x_0 \mu_0 \right), \quad E_{sol} = \mu_0 \xi_{sol} \left(\frac{m_0}{\mu_0}, x_0 \mu_0 \right) \quad (20)$$

The ratios $(-\beta/\alpha)$ of coefficient amplitudes corresponding to which these minima are obtained are exhibited in Fig. 2 as functions of the mass ratio (m_0/μ_0) . The quantity $|\beta/\alpha|$ monitors the relative probability of finding the system in the excited configuration (fluctuation) as opposed to the ground-state configuration. It is seen that as the ratio (m_0/μ_0) increases, i.e. as the classical meson becomes much heavier than the classical soliton, such relative probabilities approach 1, i.e. the systems "spend half of the time" in their excited configuration. On the other hand, these excited configurations do not appear to play a significant role for $m_0/\mu_0 \lesssim 20$. For $m_0/\mu_0 \gtrsim 20$, as fluctuations become important, the classical picture manifestly breaks down. It will be convenient to refer to the limits $m_0/\mu_0 \rightarrow 0$, $m_0/\mu_0 \rightarrow \infty$ as the classical and quantum limits, respectively.

The dimensionless quantities ξ_{vac} and ξ_{sol} as functions of $(x_0 \mu_0)$ and for fixed values of the ratio m_0/μ_0 are exhibited in Fig. 3. Not surprisingly, it is seen that soliton-antisoliton (virtual) pairs like to correlate at distances of the order of the soliton Compton wavelength^{*)}. It is perhaps useful to think of $E(x_0)$ as an effective potential binding the soliton-antisoliton pair. $E(x_0)$ is power-behaved near the origin and approaches zero exponentially for large x_0 . In the quantum limit, this potential becomes deeper, signalling the formation of a larger and larger number of soliton-antisoliton bound states¹⁰⁾.

In Fig. 4a and b the behaviour of ξ_{sol} and ξ_{vac} and of their difference as functions of the ratio (m_0/μ_0) and for $2x_0 = 1/2\mu_0$ is exhibited. In the quantum limit the presence of fluctuations lowers the vacuum and soliton energies. After shifting the vacuum energy back to zero, the soliton is found to have been made heavier by the inclusion of fluctuations corresponding to soliton-antisoliton pairs at rest.

Coming back to our general program, let us conclude with a word about collision states and scattering. Assuming that our non-perturbative expansions over field configurations have converged to good approximations of one-particle states,

*) The presence of these pairs gives structure to soliton form factors, which in the space-like region can easily be calculated with the technique described in the last article of Ref. 1. After analytic continuation to the time-like region, these form factors will be a source of information about the meson spectrum.

in the absence of long-range forces, collision states corresponding at a certain time to two widely separated particle wave packets can easily be constructed. For theories with conventional cluster decomposition^{*)}, we would express such collision states as tensor products of one-particle states such as (8):

$$|S\rangle_N \otimes |S'\rangle_N = \frac{1}{\sqrt{N}\sqrt{N'}} \sum_{n,m} a_n a'_m |f_n + f'_m, g_n + g'_m\rangle \quad (21)$$

For scattering calculations, this representation of collision states as a sum over configurations could then play a complementary role to Feynman's "sum over histories" prescription, by specifying field configurations and associated amplitudes as histories begin. This would simplify the conventional functional integral approach considerably by enabling one to calculate directly physical on-shell amplitudes rather than unphysical Green's functions. Of course, functional integrals corresponding (at least) to each pair of in-going and out-going configurations would still have to be evaluated, which needless to say, would generally be a formidable task.

In the light of this, it might be worth considering the drastic short cut implied by the following semi-classical approximation¹¹⁾

$$e^{-i\mathcal{H}t} |f, g\rangle \approx |f(t), g(t)\rangle \quad (22)$$

where $f(t)$ and $g(t)$ denote the time-dependent configuration obtained by solving the classical field equations with the initial conditions specified by f and g . The semi-classical ansatz (22), coupled with the representation (21) for particle collision states, generates a hybrid (quantum-classical) approximation to S-matrix elements within particle collision states. In this approximation, quantum fluctuations are taken into account to an arbitrarily high order in the description of particle vertices, Eq. (21), but are neglected in the time evolution of the states, Eq. (22), which retains only the minimal zero-point fluctuations, carried by coherent states, around the classical path. The mutilation implicit in Eq. (22) destroys unitarity and the group property of time translations away from the classical limit. In spite of this, the approximation based on Eqs. (21) and (22) may still prove helpful in unveiling some of the intricacies of the non-linear dynamics of quantum fields.

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*) The model used in our previous discussion is not of this type, as the presence of a soliton affects field configurations everywhere in space. The necessary modification of (21) is, however, trivial.

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Figure captions

- Fig. 1 : Anharmonic oscillator potential.
- Fig. 2 : Ratio of optimal coefficient amplitudes.
- Fig. 3 : Dependence of vacuum and soliton energies on the pair separation for $m_0/\mu_0 = 33$ and $m_0/\mu_0 = 50$.
- Fig. 4 : Dependence of vacuum and soliton energies and of their difference on the ratio m_0/μ_0 for pair separations $2x_0 = 1/2\mu_0$.

FIG.1

FIG. 2

FIG. 3a

FIG. 3b

FIG. 4a

FIG. 4b