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COUPLED CLUSTER STUDIES OF CHIRAL MESON FIELD THEORIES: THE NONLINEAR SIGMA MODEL ON THE LATTICE

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1. INTRODUCTION

Since quarks are almost massless, the QCD Lagrangian has an approximate chiral symmetry which, if it were actually realised, would result in all hadrons having chiral partners of almost equal mass but opposite parity. Since this does not occur naturally, the chiral symmetry must be spontaneously broken dynamically. The physical pions are thereby interpreted as the corresponding Goldstone bosons, with a mass proportional to both the vacuum quark condensate and the quark mass.

Since pions dominate the low-energy physics of particles interacting via the strong force, much intrinsic interest focusses on their dynamics. This interest has also been reinvigorated by the work of Brown and Rho [1], which suggested that the chiral symmetry could be restored under conditions of high enough temperature or density, such as might occur in heavy-ion collisions, where the dynamical quark mass approaches zero. Nevertheless, pion dynamics is difficult to describe in terms of the original QCD Lagrangian, especially since the pion is a composite particle. For that reason it is useful to start instead with an effective Lagrangian which is compatible with the consequences of symmetry breaking, but in which the pion dynamics is still restricted by such other pertinent (approximate) symmetries as partial conservation of the axial current.

A prototype of such a model is the $O(4)$ nonlinear sigma model, in which the $O(4)$ symmetry can be broken explicitly, but where the $O(3)$ isospin sub-symmetry remains intact. In one space and one time dimension, $(1+1)$D, the model is known to be both infrared and ultraviolet divergent [2]. More generally, the short-distance behaviour must be regularised, e.g., by latticisation, and it is this latticised version of the $O(4)$ model that we study here.

After latticisation we thereby have a model theory which in $(d+1)$D is expected, for $d > 1$, to undergo a chiral phase transition at some finite critical value of the

lattice spacing. For smaller values the model is essentially one of weakly interacting (quasi-free) rotors in a disoriented (symmetric) phase which has massive excitations characterised by the quantum numbers of the free rotors. Conversely, at larger lattice spacings than the critical value, the model comprises tightly bound rotors in an aligned (symmetry-broken) phase which has strongly collective excitations with a zero mass gap.

Following the early work of Kogut *et al.* [3], most subsequent work on the latticised nonlinear sigma model has employed the Euclidean (imaginary-time) framework of the Lagrangian formulation (viz., the statistical-mechanical approach), thereby resulting in a strong correspondence with high-temperature spin models. While one can readily study the ground state and the physical phase transition within this approach, its main drawback is that excited states and other properties are more difficult to describe. Instead, in the present work, we will treat the model in the Minkowskian (real-time) framework of the Hamiltonian formulation (viz., the quantum many-body theory, QMBT, approach), with the aim of studying both ground and excited states, as well as the phase transition. Especially in view of its considerable recent successes in dealing both with spin-lattice models of interest in (antiferro)magnetism [4] and with lattice gauge theories [5], we employ here the coupled cluster method (CCM) of QMBT. For a survey of the method and its wide array of applications, the interested reader is referred to Ref. [6]. For a fuller version of the present work the reader is also referred to Ref. [7].

2. THE LATTICISED $O(4)$ NONLINEAR SIGMA MODEL

The original continuum version of the $O(4)$ nonlinear sigma model is defined in $(3+1)$D by the Lagrangian density,

$$\tilde{\mathcal{L}} = \frac{f_\pi^2}{4\hbar c} \mathrm{Tr}\left(\partial_\mu U \partial^\mu U^\dagger\right) \quad , \tag{1}$$

where f_π ($\approx 92\,\mathrm{MeV}$) is the pion decay constant, and $U = U(x_\mu)$ is an SU(2) matrix-valued field of 2×2 unitary matrices,

$$U = \exp(-i\vec{\tau}\cdot\vec{\Pi}/f_\pi) \quad , \tag{2}$$

embodying the pion field $\vec{\Pi} = \vec{\Pi}(x_\mu)$, in terms of the usual Pauli (isospin) matrices, $\vec{\tau} \equiv (\tau^x, \tau^y, \tau^z)$. The field U may also be expressed in the form,

$$U = n_4 \mathbb{1} + i\vec{\tau}\cdot\vec{n} \quad , \tag{3}$$

and the unitarity condition, $U^\dagger U = \mathbb{1}$, is then equivalent to the constraint that $n_4^2 + \vec{n}^2 = 1$, namely that $\hat{n} = \hat{n}(x_\mu) \equiv (\vec{n}, n_4)$ is a 4D unit vector. The Lagrangian is thereby equivalently expressed in $(d+1)$D as

$$\tilde{L} = \frac{f_\pi^2}{2\hbar c} \int d^d x \left[\frac{1}{c^2}\frac{\partial \hat{n}}{\partial t}\cdot\frac{\partial \hat{n}}{\partial t} - \vec{\nabla}\hat{n}\cdot\vec{\nabla}\hat{n}\right] \equiv \tilde{T} - \tilde{V} \quad , \tag{4}$$

where f_π has dimensions (energy) $\times$ (length)$^{(3-d)/2}$.

The d spatial dimensions are now discretised onto the lattice sites of an N^d cube (with $N \to \infty$), with lattice spacing a. The fundamental field $\hat{n}(\vec{x},t)$ is thus discretized to $\hat{n}(\vec{x}_i,t)$ on lattice sites i at positions $\vec{x}_i$. The "kinetic energy" term, $\tilde{T}$, in Eq. (4) thus simply becomes

$$\tilde{T} = \frac{1}{2}\frac{f_\pi^2 a^d}{\hbar c^3}\sum_{\mathbf{i}} \frac{d\hat{n}_\mathbf{i}}{dt}\cdot\frac{d\hat{n}_\mathbf{i}}{dt} \quad . \tag{5}$$

Apart from the unitarity constraint, Eq. (5) simply represents a sum of single-particle energies of the form $\frac{1}{2}m(dx/dt)^2$, with $x \to \hat{n}_\mathbf{i}$ a 4D "position" vector and $m \to f_\pi^2 a^d/\hbar c^3$ the "mass". Without the constraint this would immediately yield the usual quantised form $p_x^2/2m$, with $p_x = -i\hbar\partial/\partial x$. Imposition of the constraint simply implies that the motion is restricted to the surface of the unit sphere in 4D. The radial part of the subsequent 4D Laplacian operator is thereby constrained to disappear, resulting in the final form

$$\tilde{T} = \frac{1}{2}\frac{\hbar^3 c^3}{f_\pi^2 a^d}\sum_{\mathbf{i}} \vec{I}_\mathbf{i}^{\,2} \quad , \tag{6}$$

in terms of the 4D angular momentum operator $\vec{I}^2$.

Similarly, in the "potential energy" term, $\tilde{V}$, in Eq. (5) the latticisation replaces the spatial derivatives by finite differences,

$$\begin{aligned}\nabla_k\hat{n}_\mathbf{i}\cdot\nabla_k\hat{n}_\mathbf{i} &\longrightarrow \frac{1}{a^2}\left[\hat{n}(\vec{x}_i + a\hat{e}_k) - \hat{n}(\vec{x}_i)\right]^2 \\ &= \frac{2}{a^2}\left[1 - \hat{n}(\vec{x}_i)\cdot\hat{n}(\vec{x}_i + a\vec{e}_k)\right] \quad , \end{aligned} \tag{7}$$

where $\hat{e}_k$ is a unit lattice vector in the k th direction.

We thus arrive at the final form,

$$\tilde{V} = \frac{f_\pi^2 a^{d-2}}{\hbar c}\sum_{\langle\mathbf{ij}\rangle}(1 - \hat{n}_\mathbf{i}\cdot\hat{n}_\mathbf{j}) \quad , \tag{8}$$

where the sum on $\langle\mathbf{ij}\rangle$ runs over all nearest-neighbour pairs, counting each pair (or lattice link) once only.

The resulting latticised $O(4)$ nonlinear sigma model Hamiltonian is thus

$$\tilde{H} = \frac{(\hbar c)^3}{f_\pi^2 a^d}\left[\frac{1}{2}\sum_{\mathbf{i}}\vec{I}_\mathbf{i}^{\,2} + \left(\frac{f_\pi a^{(d-1)/2}}{\hbar c}\right)^4\sum_{\langle\mathbf{ij}\rangle}(1 - \hat{n}_\mathbf{i}\cdot\hat{n}_\mathbf{j})\right] \quad , \tag{9}$$

which is just the Hamiltonian of a system of 4D symmetric tops (or quantum rotors) with a nearest-neighbour interaction tending to align them. Henceforth, we drop the overall energy scale factor, $(\hbar c)^3/f_\pi^2 a^d$, and study the dimensionless Hamiltonian

$$H = \frac{1}{2}\sum_{\mathbf{i}}\vec{I}_i^{\,2} + \lambda\sum_{\langle\mathbf{ij}\rangle}(1 - \hat{n}_\mathbf{i}\cdot\hat{n}_\mathbf{j}) \quad , \tag{10}$$

in terms of the dimensionless coupling constant, $\lambda \equiv \left(f_\pi a^{(d-1)/2}/\hbar c\right)^4$. We shall study this Hamiltonian in $d = 1, 2$, and 3 spatial dimensions. In each case we consider varying the lattice spacing a, and hence consider λ a free parameter, even though in the (singular) case $d = 1$ the parameter λ is independent of a.

Finally, we note that our definition of the angular momentum operators in Eq. (10) employs the convention related to the $O(4)$ symmetry. The reader should beware that an alternative convention related to the $SU(2)$ isospin symmetry introduces additional factors of one-half into the definition of the components of $\vec{I}$. Thus, in our own convention, for the more general $O(N)$ theory, the Gegenbauer polynomials $C_n^{(N-2)/2}(\cos\theta)$ are eigenfunctions of $\vec{I}^2$ with corresponding eigenvalues given by $n(n+N-2)$. Thus, for the $N = 4$ case studied here, the eigenvalues of the operator $\vec{I}^2$ are $n(n+2) \equiv 4j(j+1)$ when $n = 2j$, and where j is the usual integral or half-integral $SU(2)$ quantum number.

The $O(4)$ unit vectors $\hat{n}_\mathbf{i}$ may be parametrised in terms of spherical coordinates as

$$\hat{n} = (\sin\theta\sin\phi\sin\chi, \sin\theta\sin\phi\cos\chi, \sin\theta\cos\phi, \cos\theta) \quad , \tag{11}$$

with $0 \le \theta < \pi$, $0 \le \phi < \pi$, and $0 \le \chi < 2\pi$. The kinetic energy operator $\frac{1}{2}\vec{I}^2$ may be derived from the generalised angular momentum operators,

$$L_{kl} \equiv -i(n_k\partial_{n_l} - n_l\partial_{n_k}) \quad , \tag{12}$$

where $k, l = 1, 2, \cdots, N$ for the general $O(N)$ case, with $N \ge 2$. Specifically, it may be related to the $O(N)$ Casimir invariant,

$$\vec{I}^2 = \sum_{k<l} L_{kl}^2 \quad . \tag{13}$$

For many purposes we need only the θ-dependent part of $\vec{I}^2$, in which case we have

$$\vec{I}^2 \longrightarrow -\partial_\theta^2 - (N-2)\cot\theta\,\partial_\theta = -\frac{1}{\sin^{N-2}\theta}\partial_\theta\left(\sin^{N-2}\theta\,\partial_\theta\right)$$

$$= -(1-\cos^2\theta)\partial_{\cos\theta}^2 + (N-1)\cos\theta\,\partial_{\cos\theta} \quad . \tag{14}$$

In particular, in two-body approximations of the CCM SUB2 type discussed below, we need only those parts of the Hamiltonian H in Eq. (10) which depend on the relative variables $\theta_{\mathbf{ij}} \equiv \cos^{-1}(\hat{n}_\mathbf{i}\cdot\hat{n}_\mathbf{j})$. In such cases,

$$H \longrightarrow \sum_{[\mathbf{ij}]} -\frac{1}{\sin^2\theta_{\mathbf{ij}}}\partial_{\theta_{\mathbf{ij}}}\left(\sin^2\theta\,\partial_{\theta_{\mathbf{ij}}}\right) + \lambda\sum_{\langle\mathbf{ij}\rangle}(1-\cos\theta_{\mathbf{ij}}) \quad , \tag{15}$$

where the sum on $[\mathbf{ij}]$ now runs over *all* pairs of lattice sites $\mathbf{i}$ and $\mathbf{j}$, counting each pair once. We note that the factor of one-half in the kinetic energy term in Eq. (10) is missing from Eq. (15), since the operator $\sum_\mathbf{i}\vec{I}_\mathbf{i}^2$ acts twice on each relative coordinate $\theta_{\mathbf{ij}}$, once from each lattice site.

3. THE CCM FOR CLASSICAL SPIN MODELS

The standard operatorial formulation of the CCM [6] is widely acknowledged to be one of the most widely applicable, most powerful, and numerically most accurate at attainable levels of implementation, of all microscopic QMBT methods. Although it has also been applied by us [7] to the latticised nonlinear sigma model, we report here only on results obtained via an alternative functional formulation which was earlier applied to lattice gauge theories [5].

The key ingredient in the functional formulation is the parametrisation of the many-body ground-state ket and bra wave functions in the respective forms,

$$\langle\{r\}|\Psi\rangle = \exp[S(\{r\})] \ , \tag{16a}$$

$$\langle\tilde{\Psi}|\{r\}\rangle = [1+\tilde{S}(r)]\exp[-\tilde{S}(\{r\})] \ , \tag{16b}$$

where $|\{r\}\rangle$ is some suitably chosen complete and normalised set of many-body wave functions, such that

$$\int d\{r\}\,|\{r\}\rangle\langle\{r\}| = \mathbb{1} \ . \tag{17}$$

This approach is naturally suited to lattice Hamiltonians, where $|\{r\}\rangle$ can simply be chosen as a direct product of complete states at each lattice site. Thus, for our present $O(4)$ model application, we choose

$$|\{r\}\rangle \longrightarrow |\{\hat{n}\}\rangle = \prod_{\mathbf{i}} |\hat{n}_{\mathbf{i}}\rangle \ , \tag{18}$$

where the state $|\hat{n}_{\mathbf{i}}\rangle$ is the standard 4D spherical-coordinate representation specified in Eq. (11), at lattice site $\mathbf{i}$. We now introduce a (bi-)variational energy functional,

$$\langle\tilde{\Psi}|H|\Psi\rangle \equiv J[S,\tilde{S}] = \int d\{r\}\int d\{r'\}\,[1+\tilde{S}(\{r\})]\exp[-S(\{r\})]$$
$$\times\langle\{r\}|H|\{r'\}\rangle\exp[S(\{r'\})] \ . \tag{19}$$

The ground-state wave functions and energy are then obtained from the (bi-)variational principle $\delta J = 0$, subject to the normalisation constraint,

$$\langle\tilde{\Psi}|\Psi\rangle = 1 \quad\Longrightarrow\quad \int d\{r\}\,\tilde{S}(\{r\}) = 0 \ . \tag{20}$$

Approximations in this functional form of the CCM are now made by restricting the class of trial many-body lattice functions $S(\{\hat{n}\})$ and $\tilde{S}(\{\hat{n}\})$. For example, the simplest (so-called LSUB2) approximation massively restricts S and $\tilde{S}$ to include only nearest-neighbour pairwise correlations,

$$S_{\mathrm{LSUB2}}(\{\hat{n}\}) = \sum_{\langle\mathbf{ij}\rangle} S(\theta_{\mathbf{ij}}); \quad \tilde{S}_{\mathrm{LSUB2}}(\{\hat{n}\}) = \sum_{\langle\mathbf{ij}\rangle} \tilde{S}(\theta_{\mathbf{ij}}), \tag{21}$$

where $\cos\theta_{ij} \equiv \hat{n}_i \cdot \hat{n}_j$, as before. By making use of Eq. (15), the LSUB2 variational functional takes the form

$$J_{\mathrm{LSUB2}}[S,\tilde{S}] = N_l \frac{2}{\pi}\int_0^\pi d\theta \, \sin^2\theta[1+\tilde{S}(\theta)][-S''-2\cot\theta\, S'-S'^2+\lambda(1-\cos\theta)] \ , \quad (22)$$

where N_l is the number of (nearest-neighbour) links on the lattice.

The more general SUB2 approximation, results from which we cite in Sec. 4, restricts S and $\tilde{S}$ to include *all* pairwise correlations,

$$S_{\mathrm{SUB2}}(\{\hat{n}\}) = \sum_{[ij]} S_{\chi_{i-j}}(\theta_{ij}); \quad \tilde{S}_{\mathrm{SUB2}}(\{\hat{n}\}) = \sum_{[ij]} \tilde{S}_{\chi_{i-j}}(\theta_{ij}) \ , \quad (23)$$

where the integer irrep suffix χ_{i-j} labels each *distinct* member of each independent set of pairwise correlation functions, after taking into account functions which are identical under the lattice symmetries (i.e., translations, rotations, and reflections). The evaluation of the kinetic energy part of the SUB2 energy functional of Eq. (19) is more difficult than in the LSUB2 case, since the two differentiations can now also link two correlation functions S on different pairs of sites $(\mathbf{i},\mathbf{j})$. Nevertheless, one can also fairly readily derive the SUB2 analogue of its LSUB2 counterpart in Eq. (22). Full details are given elsewhere [7].

In view of this added complexity of the SUB2 case, the resulting variational equations are best obtained and solved by expanding the sets $\{S_{\chi_{i-j}}(\theta)\}$ and $\{\tilde{S}_{\chi_{i-j}}(\theta)\}$ in an appropriate set of complete functions of the variable θ (or $\cos\theta$). Since in the weak-coupling limit ($\lambda \to 0$) the eigenstates of H are simply the Gegenbauer polynomials, this is a particularly appealing set, and the one we choose for our numerical results. Furthermore, we note that the normalisation constraint of Eq. (20) is then also trivial to impose in terms of such an expansion. In practice the SUB2 approximation is implemented as a SUB2–n–m sequence in which we truncate both on the number n of distinct pairwise correlations retained from the otherwise infinite set, and on the number m of (Gegenbauer polynomial) basis functions in which each is expanded. In practice we find extremely rapid convergence in the index m, with all pairwise correlation functions typically being very well approximated with just three basis functions. We comment further in Sec. 4 on the dependence of the results on the truncation index n.

Finally, we may also study the collective excitations within the functional form of the CCM by employing a small-fluctuation RPA-type expansion around the above (approximated) stationary ground state resulting from $\delta J = 0$. After allowing the many-body correlations to be time-dependent we define an action functional,

$$\int_0^T dt \, \langle\tilde{\Psi}|(i\partial_t - H)|\Psi\rangle \equiv \mathcal{A}[S,\tilde{S}]$$

$$= -i\int_0^T dt \int d\{r\}\, \dot{\tilde{S}}(\{\hat{n}\},t) S(\{\hat{n}\},t) - \int_0^T dt\, J[S,\tilde{S}] \ . \quad (24)$$

An expansion of the SUB2–n–m correlations functions in terms of m Gegenbauer polynomials yields an action functional of standard canonical form. The variational

principle, $\delta\mathcal{A} = 0$, thereby results in (classical) canonical forms of the equations of motion in terms of an energy functional $J_{\mathrm{SUB2}-n-m}[S, \tilde{S}]$. By expanding around the stationary ground-state solution (from $\delta J_{\mathrm{SUB2}-n-m} = 0$), and retaining second-order terms, the resulting small-amplitude limit gives the collective excitations as the normal modes. In particular, we are interested in the lowest excitation energy, which is simply the smallest eigenvalue of the resulting dynamic matrix.

4. RESULTS

In Figs. 1 and 2 we show, respectively, the ground-state energy per link, E/N_l, and the lowest excitation energy, E_x, as functions of the coupling constant, for the latticised $O(4)$ nonlinear sigma model Hamiltonian of Eq. (10) in $d = 1, 2$, and 3 space dimensions. The results are obtained in the SUB2–n–m approximation to the functional form of the CCM described in Sec. 3. In all cases shown, the values of the truncation indices n and m are large enough for convergence to have been demonstrably obtained on the scale of the figures. In practice, convergence (in the index n) of the number of distinct pairwise correlations retained is tested by retaining, at each step, all correlations between pairs up to a given distance L apart on the lattice, and examining the behaviour of the results as functions of L.

The most striking feature of Fig. 1 is the presence of a critical point, λ_c, beyond which (i.e., for $\lambda > \lambda_c$) no ground-state solution is found. More precisely, for a given truncation level n (and m), the ground-state solutions are double-valued for $\lambda < \lambda_c$, with the two branches coinciding at $\lambda = \lambda_c$. As the truncation index n is increased, the two branches lie closer and closer to one another, and in Fig. 1 are indistinguishable from each other. In all cases one of the two branches is "unphysical" in the sense that it does not connect directly with the known perturbative "physical" branch at small values of λ. We interpret the appearance of the critical points, λ_c, as possible indicators of a quantum phase transition beyond which our solutions break down. We also note that near λ_c convergence in n (or, equivalently, L) is slowest, as might be expected near a phase transition at which the correlation length diverges to infinity. The actual value of the critical point, $\lambda_c(L)$, for truncation at a given range L is found heuristically to be accurately fitted by a form, $\lambda_c(L) = \lambda_c(\infty) + c/L^2$. The corresponding SUB2 values of the critical point are at $\lambda_c(\infty) \approx 1.927$, 0.827, and 0.536, respectively for the model in $(1+1)$, $(2+1)$, and $(3+1)$ dimensions. Since no physical phase transition can actually occur in (1+1)D [8], and since our observed value of λ_c is so high in this case, we expect that the existence of our (1+1)D critical point is not robust against the inclusion of the many-body correlations missing from our SUB2 calculations. Although the stability of the critical points in (2+1)D and (3+1)D is presently unknown, we expect them to survive to higher orders.

That the critical point at λ_c represents a phase transition is lent considerable credence by the fact that the lowest excitation energy (or mass gap), E_x, approaches zero at this point, as is clearly seen to be the case from Fig. 2. Thus, a collective mode becomes soft as $\lambda \to \lambda_c$. In accordance with the discussion in Sec. 1 we imagine that in the chirally symmetric mode, which exists for $\lambda < \lambda_c$, we get a macroscopic occupation of this collective mode as $\lambda \to \lambda_c$; and for $\lambda > \lambda_c$ we expect that the zero mass gap is retained in the (aligned) phase in which chiral symmetry is broken.

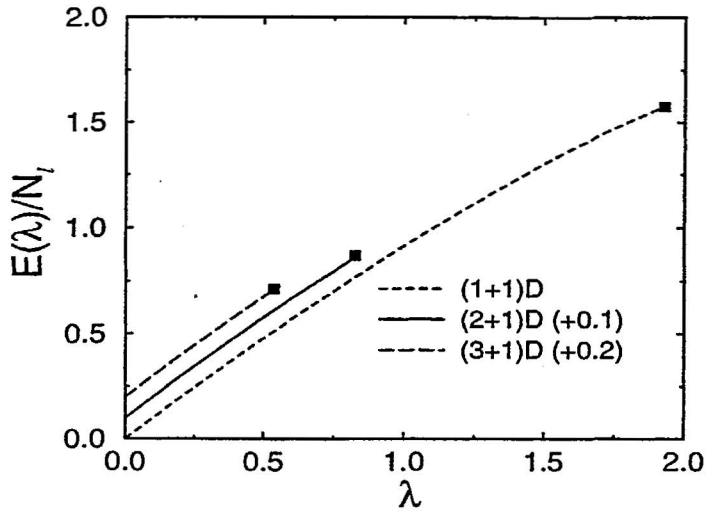

Figure 1. The ground-state energy per link for the latticised $O(4)$ nonlinear sigma model in $(d+1)$D, using the SUB2–n–m approximation to the functional form of the CCM. Termination points are denoted by the solid squares. The results in $(2+1)$D and $(3+1)$D are shown vertically offset by the addition of 0.1 and 0.2, respectively, for ease of display.

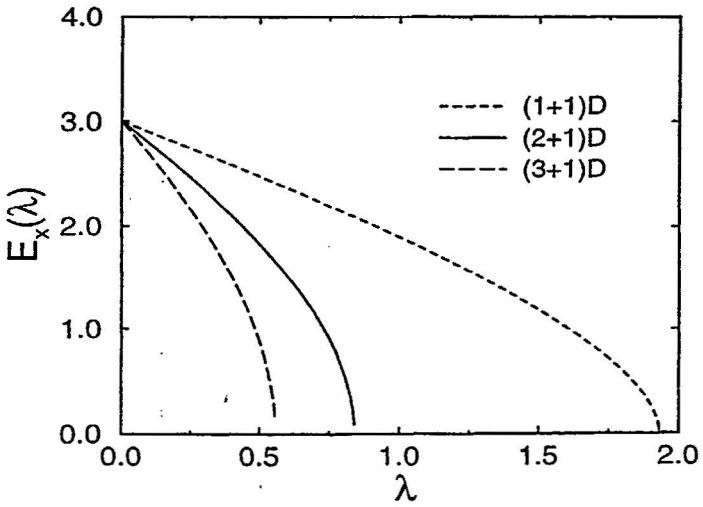

Figure 2. The lowest excitation energy of the latticised $O(4)$ nonlinear sigma model in $(d+1)$D, using the RPA method based on the SUB2–n–m approximation to the functional form of the CCM.

5. SUMMARY AND CONCLUSIONS

We have shown that latticised chiral meson field theories may profitably be studied in the Hamiltonian QMBT formulation, where they are essentially "classical" spin models. In particular, we have shown that for the $O(4)$ nonlinear sigma model, the functional form of the CCM readily yields clear evidence of a chiral phase transition at some critical value, λ_c, of the coupling constant, near which a collective mode becomes soft. We note too that similar calculations have also been performed by us [7] in the operatorial form of the CCM, with numerically very similar results.

Our calculations to date have been done at the SUB2 level in which only two-body correlations are included. In principle, we could extend the SUB2 scheme to its SUBn counterpart in which all many-body correlations between the $O(4)$ quantum rotors on up to n sites at a time are retained. However, since many-body orthogonal polynomials are not so simple to define, we have not yet extended the functional formulation of the CCM to SUBn schemes with $n > 2$. Doubtless, however, it will be of considerable interest to do so, particularly so as to examine how robust are our SUB2 results against the inclusion of n-body correlations with $n > 2$. It will also be of great interest to attempt to extend our results into the region $\lambda > \lambda_c$ where chiral symmetry is broken.

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