A SIMPLE NUMERICAL METHOD FOR CHECKING ANALYTICAL CHIRAL BAG CALCULATIONS

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A scheme for numerical calculation of certain values in the Chiral Bag Model, obtained independently by means of asymptotic expansions, is presented. The method was employed in the case of the moments of the baryon number density originating from the vacuum polarization, serving as a cross check for the correctness of analytical calculations.

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In the Chiral Bag Model [1] baryons are portrayed as consisting of free masless quarks confined inside a spherical bag and coupled to the external mesonic field constituting a Skyrme soliton[1]. The boundary condition for the quark field is

$$-i\vec{\gamma}\cdot\hat{n}\Psi(r)\,|_{r=R} = \exp\left(i\Theta\vec{\tau}\cdot\hat{n}\gamma_5\right)\Psi(r)|_{r=R}, \tag{1}$$

where R is the radius of the bag, $\hat{n} = r/R$ and Θ is a real number describing the strength of the classical pion field at the surface of the bag. The components of the vector $\vec{\tau}$ are the Pauli matrices acting in isospin space.

The coupling at the surface leads to the asymmetry between virtual quarks and antiquarks, what results in non-zero contribution to many quantum numbers which comes

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[1] for a detailed description of this model and the calculations involved see [2–3]. Notation and conventions used here are the same as in [2].

from the polarization of vacuum. These quantites are defined by the sum

$$Q_{\text{vac}} = -\tfrac{1}{2} \sum_{\{E\}} \text{sign}\,(E) Q(E), \tag{2}$$

where Q is the vacuum expectation value of a symmetrized operator $\frac{1}{2}[\Psi^+, \hat{Q}\Psi]$ and energy levels E are found by solving free, masless Dirac equation with the boundary condition (1). This sum can be divergent and is regularized using the Poisson method

$$Q_{\text{vac}} = -\tfrac{1}{2} \lim_{t \to 0+} \sum_{\{E\}} \text{sign}\,(E) Q(E) e^{-t|E|}. \tag{3}$$

The energy levels are labelled using the following quantum numbers: n, K, M, sign (E), P and ε. The number n labels radial excitations, K and M are connected with the operator $\boldsymbol{K} = \boldsymbol{I} + \boldsymbol{J}$, where $\boldsymbol{I}$ and $\boldsymbol{J}$ are angular momentum and isospin operators respectively. $K(K+1)$ is an eigenvalue of $\boldsymbol{K}^2$ and M an eigenvalue of the third component of $\boldsymbol{K}$. All energy levels are degenerate with respect to M because of the symmetry of the problem under SU(2) rotations in K-space. P is the space parity. From now on sign (E) will be denoted by κ. For $K > 0$ there are two distinct solutions with the same n, K, M, κ and P; and thus ε is introduced as an additional index, necessary to remove ambiguity.

It is very useful to introduce a special symbol for the average of any expression Q [4]:

$$\langle Q \rangle = \begin{cases} \frac{1}{8} \sum_{\kappa, P, \varepsilon} \kappa Q(\kappa, P, \varepsilon), & \text{when} \quad K > 0; \\ \frac{1}{4} \sum_{\kappa, P} \kappa Q(\kappa, P), & \text{when} \quad K = 0. \end{cases} \tag{4}$$

The terms occurring in (3) have alternating signs and cancel each other partially. Thus the convergence of the series (3) is more obvious when rewritten using averages, where all cancellations are already performed. Moreover, due to existing symmetries of the energy levels, the functional form of the averages is much simpler than that of its components. Employing (4) and splitting the $K = 0$ and $K > 0$ parts we rewrite (3) as

$$Q_{\text{vac}} = Q_{K=0} + Q_{K>0} = -2 \lim_{t \to 0+} \sum_{n=1}^{\infty} \langle Q_n e^{-t x_n} \rangle - 8 \lim_{t \to 0+} \sum_{n,\nu} \langle \nu Q_{n\nu\varepsilon} e^{-t x_{n\nu\varepsilon}} \rangle, \tag{5}$$

where we took advantage of the degeneracy with respect to M. The dimensionless quantities $x_n(\Theta)$ and $x_{n\nu\varepsilon}(\Theta)$ denote the absolute values of the eigenenergies multiplied by the bag radius R; Q_n and $Q_{n\nu\varepsilon}$ denote the quantities evaluated in the stationary states with quantum numbers n and $n\nu\varepsilon$ respectively, and $\nu = K + 1/2$.

We will concentrate on the quantities for $K > 0$, since they will serve as a better example for the application of our method because the formulae involved are much more complicated. The sum defining $Q_{K>0}$ in (5) can be rewritten in such a way that all divergent terms are extracted and calculated analytically (this part, called anomalous, will be denoted by $\mathscr{A}_{K>0}$) and in the remaining part (called regular and denoted by $\mathscr{R}_{K>0}$) we can directly set $t = 0$. For further details of this calculation see [2].

We have used the Euler-Maclaurin summation formula for performing summation of the anomalous part, obtaining

$$Q_{K>0} = \mathscr{A}_{K>0} + \mathscr{R}_{K>0}$$

$$= \overline{\mathscr{A}}_{K>0} - \frac{8}{\pi} \int_0^{\pi/2} d\beta_0 \tan^2 \beta_0 \langle m_3^{(2p)} \rangle \ln \cos \beta_0 - 8 \sum_{\nu} \sum_{n} \langle \nu M_{n\nu\varepsilon}^{(2p)} \rangle, \tag{6a}$$

where

$$\overline{\mathscr{A}}_{K>0}$$

$$= \frac{8}{\pi} \int_0^{\pi/2} d\beta_0 \sin^2 \beta_0 [(\langle m_2^{(2p)} a_0 \rangle + \langle m_1^{(2p)} a_1 \rangle + \langle m_0^{(2p)} a_2 \rangle)/\cos \beta_0 - m_0^{(2p)} \langle a_0 a_1 \rangle]. \tag{6b}$$

The functions a_k and $m_k^{(2p)}$ are defined as the coefficients in asymptotic expansions for the energy levels

$$x_{n\nu\varepsilon} \sim \frac{\nu}{\cos \beta_0} + \sum_{k=1}^{\infty} \frac{a_k(\beta_0, \varepsilon; \Theta)}{\nu^k}, \tag{7}$$

and the corresponding quantities Q

$$Q_{n\nu\varepsilon} \sim \sum_{k=1}^{\infty} \frac{m_k(\beta_0, \varepsilon; \Theta)}{\nu^k}, \tag{8}$$

where β_0 is found as the only solution of the equation

$$\nu(\tan \beta_0 - \beta_0) = n\pi, \tag{9}$$

satisfying $0 < \beta_0 < \pi/2$. The analytical formulae for the averages existing in (6) were calculated and are given in [3].

The above calculations were performed in the case of the even moments of the distribution of the baryon charge M_{2p}^{vac} [3]. $(2p)$ will denote the quantities connected with the $2p$-th moment. The calculations are straightforward but lenghty and the analytical expressions involved are rather complicated (cf. Appendix A in [3]). Thus it is very important to ensure the correctness of the results. One possible cross-check is suggested by the fact that

$$\int_0^{\pi/2} d\beta_0 \tan^2 \beta_0 \langle m_3^{(2p)} \rangle = 0, \tag{10}$$

is required to ensure that there is no logarithmic divergence in $M_{(2p)}^{\text{vac}}$. This test, which is

highly non-trivial, considering complexity of the formulae involved, was passed satisfactorily.

We have also used another, more direct test for the correctness of the formulae for the averages. It relies on numerical calculation of the expectation values of some operators. Let us consider the expectation values of the following operators: $\hat{r}^{2p}$, $\hat{r}^{2p}\,|\hat{H}|$, $\hat{r}^{2p}\,|\hat{H}|^2$. If we evaluate the average (4) using these expectation values then, for certain fixed ν, we can represent the results using inverse powers of ν

$$\langle M_{n\nu\varepsilon}^{(2p)}\rangle = \frac{C_3^M}{\nu^3} + \frac{C_4^M}{\nu^4} + \dots,$$

$$\langle M_{n\nu\varepsilon}^{(2p)} x_{n\nu\varepsilon}\rangle = \frac{C_2^{Mx}}{\nu^2} + \frac{C_3^{Mx}}{\nu^3} + \dots,$$

$$\langle M_{n\nu\varepsilon}^{(2p)} x_{n\nu\varepsilon}^2\rangle = \frac{C_1^{Mx^2}}{\nu} + \frac{C_2^{Mx^2}}{\nu^2} + \dots. \tag{11}$$

It should be noted that the leading coefficients in this expansion are related to a_k and $m_k^{(2p)}$ from (7) and (8)

$$C_3^M(\beta_0; \Theta) = \langle m_3^{(2p)}\rangle,$$

$$C_2^{Mx}(\beta_0; \Theta) = \langle m_2^{(2p)} a_0\rangle + \langle m_1^{(2p)} a_1\rangle + \langle m_0^{(2p)} a_2\rangle,$$

$$C_1^{Mx^2}(\beta_0; \Theta) = 2\langle m_0^{(2p)} a_0 a_1\rangle. \tag{12}$$

The further coefficients C can be similarly expressed by combinations of a_k and $m_k^{(2p)}$ for larger k. Since all r.h.s. of (12) are given by analytic formulae the simplest way of checking their correctness is to omit all but leading terms (that is these with the lowest power of ν) in the r.h.s. of (11) and to compare them with the numerically calculated averages in the l.h.s. of (11). The accuracy of this approach is limited by the following facts:

— ν must be quite large, since the terms omitted in transition from (11) to (12) are proportional to $1/\nu$,

— for a fixed ν n cannot be too small, since the analytical formulae were derived using asymptotic expansions, which work correctly for high energy levels (large n).

Considering the above, it follows from (9) that the agreement between the values calculated analytically and numerically cannot be very good for small β_0.

This check was performed for all averages appearing in (6), i.e. necessary for the calculation of $\bar{\mathscr{A}}_{K>0}$. Typical results of such comparison are shown in Fig. 1. Here C_2^{Mx} (solid line) is compared with the averages computed for various K and n. The agreement is indeed very good for β_0 close to $\pi/2$ and intermediate, and becomes worse for smaller β_0. We can also see that, even for $K = 1000$, the agreement is not-so-perfect for $\beta_0 < 0.3$. This confirms our expectations and means only that the validity of this method of checking is limited to $\beta_0 \in (0.3, \pi/2)$. Nevertheless, it is a very strong confirmation of the correctness of analyt-

ical formulae for the averages. It would be very unlikely if several very complicated functions of β_0 and Θ would give correct values only for certain values of their arguments. Such possibility, however, cannot be, at this stage, completely ruled out.

A natural improvement on this method would be inclusion of the higher-order terms. In principle it is possible to do it, but the effort put into this calculation, due to the complexity of the formulae involved, would outweight the profit. It is possible, however, to

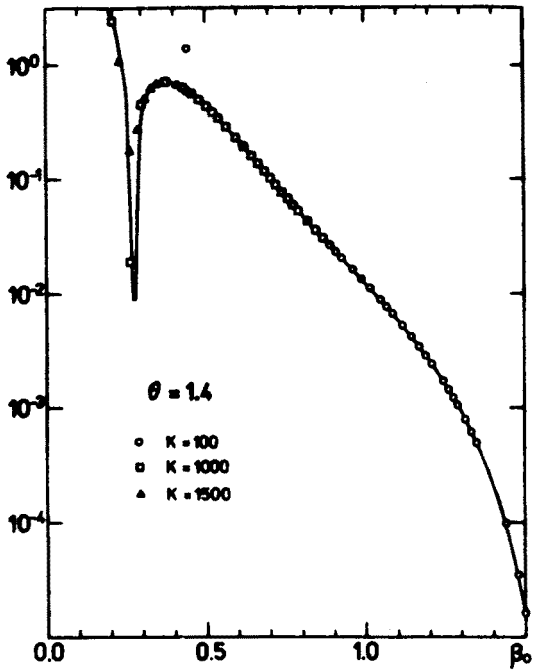

Fig. 1. C_2^{Mx} for $p = 1$ and $\Theta = 1.4$ (solid line) is compared with the results of the numerical averaging of $M_{nve}^{(2p)} x_{nve}$. Open triangles, circles, boxes and crosses denote averages obtained using $K = 100$, 200, 500 and 1000, respectively

include higher order terms implicitly, if we observe that from (9) it follows that β_0 depends only on the ratio n/v and not on n and v separately. Since coefficients C depend only on β_0 and Θ we can compute averages for two values of n and v chosen in such a way that the ratio n/v remains constant, i.e. $n/(K+1/2) = n'/(K'+1/2)$. This condition is fulfilled for instance by $n' = 3n$ and $K' = 3K+1$. Then we can eliminate the higher-order C. For example in the case of $\langle M_{nve}^{(2p)} \rangle$ we would have

$$\langle M_{nve}^{(2p)} \rangle = \frac{C_3^M}{v^3} + \frac{C_4^M}{v^4},$$

$$\langle M_{nve}^{(2p)} \rangle' = \frac{C_3^M}{v'^3} + \frac{C_4^M}{v'^4}, \tag{13}$$

from which we obtain

$$\frac{\nu^4\langle M_{nve}^{(2p)}\rangle - \nu'^4\langle M_{nve}^{(2p)}\rangle'}{\nu-\nu'} = C_3^M, \tag{14}$$

where denotes the quantities computed using n' and K'. The results of such approach for $p = 10$ and $\Theta = 1.4$ are depicted in Fig. 2. A substantial improvement in the agreement

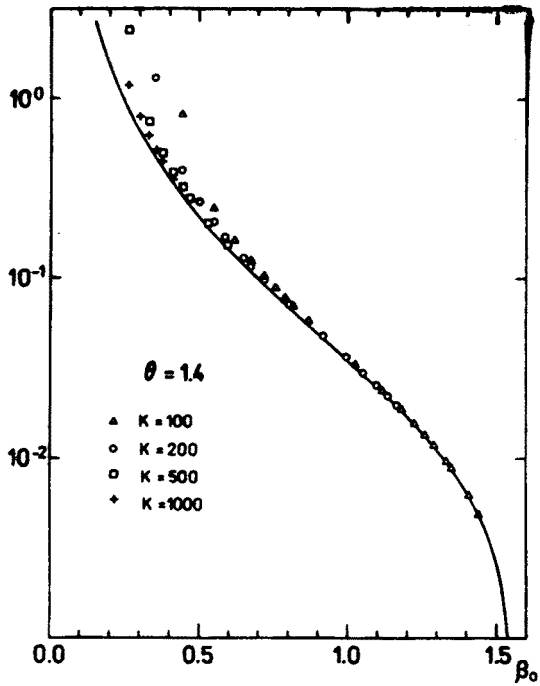

Fig. 2. C_3^M for $p = 10$ and $\Theta = 1.4$ (solid line) is compared with the results of improved numerical averaging of $M_{nve}^{(2p)}$ (formula (14)). Open circles, boxes and triangles denote averages obtained using $K = 100$, 1000 and 1500, respectively

for low values of β_0 can be seen. It should be noted that the scale is logarithmic, and that the two values agree over five orders of magnitude. The sharp dip corresponds to the change of sign.

The above calculation shows that we are able to obtain values for the quantities given in (12) using numerical method rather than analytical formulae and that both approaches give the same results with high accuracy. This means that in order to calculate some quantity, e.g. $\bar{\mathscr{A}}_{K>0}$, we do not have to calculate the integral given in (6b) analytically. Instead we can perform numerical integration using numerical estimates of the averages appearing in the integrated function. This alternative method for obtaining the solution has the virtue of being free from indulging in tedious analytical calculations.

The proposed method of integration is as follows: first we calculate function to be integrated in a sufficiently large number of values of β_0, and then we use any method for numerical integration which does not require fixed distance between points on x-axis. It is necessary since β_0 cannot be taken arbitrarily but has to satisfy (9). It should be also noted that the solutions of (9) are not evenly spaced in the interval $(0, \pi/2)$. For a fixed ν β_0 soon approaches $\pi/2$ with growing n. Thus we have at our disposal only few small

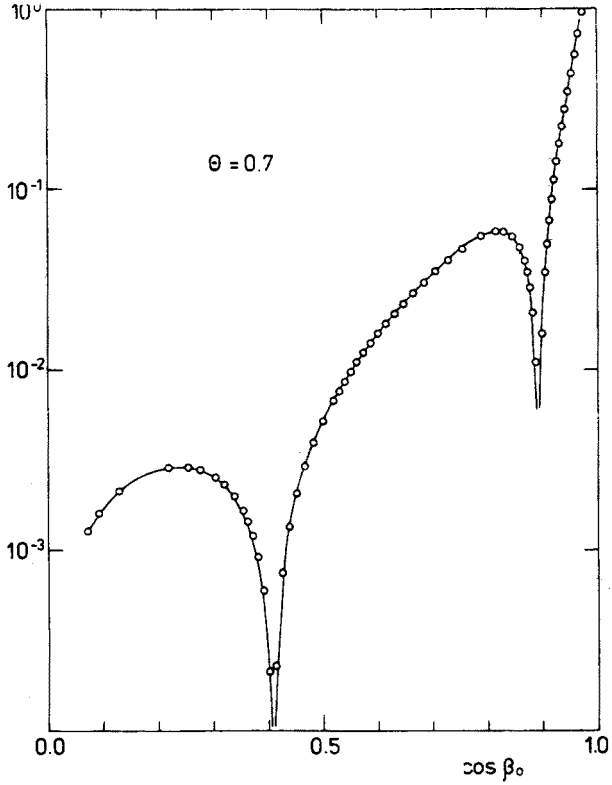

Fig. 3. $\tan^2 \beta_0 \langle m_3^{(2p)} \rangle$ as a function of $\cos \beta_0$. Open circles denote numerical values, solid line is obtained from analytical formula. For the sake of clarity of the picture only some points used for numerical calculation are actually shown. Specifically, for $\beta_0 > 0.4$, only about 1/10 of the total number of points used is depicted

β_0, corresponding to few first n. The remedy for this is to take β_0 for several ν. Moreover, in order to obtain small β_0 we must take large K, of the order of 1000 or more.

Before applying this method to the calculation of $\bar{\mathcal{A}}_{K>0}$ let us check how does it work in the case of the integral (10). The result of the integration should be 0, and therefore the area enclosed by the curve in Fig. 3, where the function to be integrated is depicted, should have its positive (i.e. above the x-axis) and negative (i.e. below the x-axis) parts equal. Examination of the Fig. 3 reveals that in order to obtain the correct result the (integrable) divergence appearing for $\beta_0 = 0$ should be treated carefully. This is done by fitting a func-

tion exhibiting divergent behaviour for $\beta_0 = 0$ to the numerical points lying close to the end of the interval and using analytical formula for its integral from the last known point to the end of the interval. If we denote the smallest β_0 available by $\beta_{\min}$ then we can calculate the integral as $\int_0^{\beta_{\min}}$ (*fitted function*) + *numerical formula using discrete points*. We have obtained the best fits using function of the form a/x^{α}, and the best fit value of α was close to 0.5.

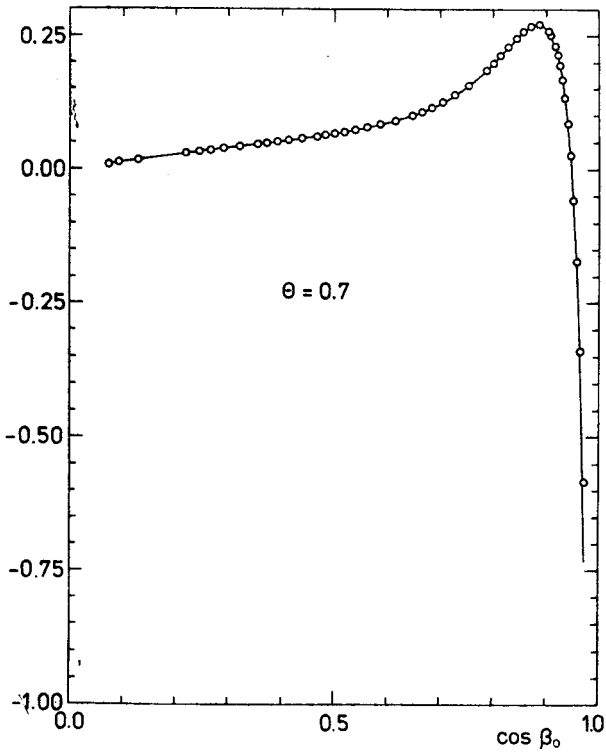

Fig. 4. $\sin^2 \beta_0 [(\langle m_2^{(2p)} a_0 \rangle + \langle m_1^{(2p)} a_1 \rangle + \langle m_0^{(2p)} a_2 \rangle)/\cos \beta_0 - m_0^{(2p)} \langle a_0 a_1 \rangle]$ as a function of $\cos \beta_0$. Open circles denote numerical values, solid line is obtained from analytical formula. Not all points actually used for calculation of the integral are plotted, see caption to Fig. 3

As far as the value of $\bar{\mathcal{A}}_{K>0}$ is concerned we employed similar method and again encountered difficulties arising from the necessity to extrapolate from the numerically calculated values to the end points of the interval. The result depends quite strongly on the type of function used for interpolation. Moreover, as it can be seen in Fig. 4, the values of the integrated function vary over five orders of magnitude in the interval of integration, what again makes fitting and extrapolation crucially dependent on the chosen functional form. It does not, however, exclude possibility of obtaining correct results.

An example of such results is presented in Fig. 5, where we plot $\bar{\mathcal{A}}_{K>0}$ as a function of Θ for $p = 5$. Comparison with exact (analytical) formula shows that the agreement is

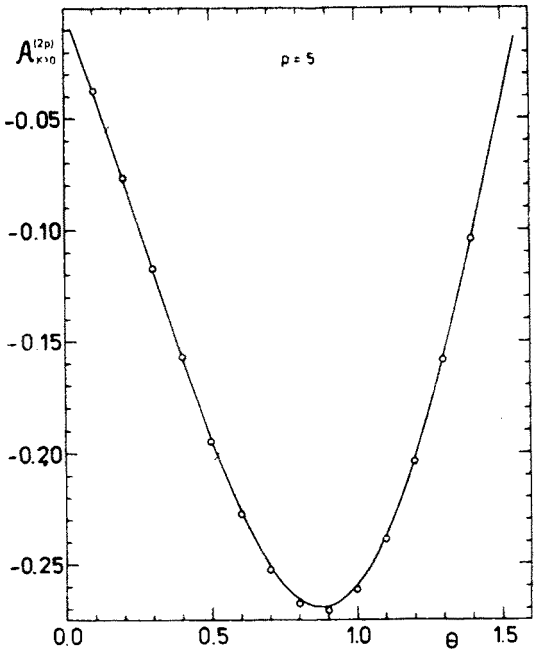

Fig. 5. $\bar{\mathscr{A}}_{K>0}$ as a function of Θ for $p = 5$. Open circles denote numerical values, solid line is obtained from analytical formula

good. Thus, the numerical method not only serves as a cross-check for the correctness of the analytical formulas, but also provides alternative method of obtaining final values.

Concluding, we have proposed a method for numerical cross-check of analytical calculations used in chiral bag calculations. This method can also be used for independent calculation of expectation values of operators.

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