Numerical study of the density of states for the bag model

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Abstract

The density of states for an extended MIT bag model is studied numerically by using a parameterized smooth representation which provides the best fit to the numerical data. It is found that the mass dependence of the surface term in the density of states agrees with that derived from multi-reflection theory calculation. The mass dependence of the curvature term in the density of states is extracted for finite values of the quark mass. The scaling properties of the data, which is assumed in the parameterization, are studied. The difference between the parameterized smooth representation determined by a best fit and the results derived from direct smoothing of the numerical data are discussed. The fluctuations in the density of states are also discussed. We provide a smooth representation of the density of states of a spherical cavity for non-relativistic particles.

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I. INTRODUCTION

Since the bag model suggested by the MIT group in the 1970s, many other bag models including the chiral bag [1], soliton bag [2] and quark-meson coupling model [3] which take the quark and meson coupling interactions into account, have been put forward with widely successful applications in nuclear physics. Recently, the bag model has been extended to include strange quarks [4,5], and has been employed to study the properties of a strangelet [6] which is believed, if it exists, to be an unambiguous signature for the formation of quark-gluon plasma [9].

To calculate the dynamical and/or thermodynamical quantities of spherical nuclei or a spherical droplet of hadronic or quark matter, in particular the strange quark matter, by means of the bag model, we must first look for the density of states (DOS) of the spherical system. The DOS of a spherical cavity in which the free particles are contained can be expressed as [10]

$$\rho(k) = \frac{dN(k)}{dk},$$

(1)
where \( N(k) \) is the total number of particle states. In general, the quantum states are discrete and \( N(k) \) is a summation of discontinuous states. But in practical calculation, a continuous representation of the DOS is needed for changing the summation to an integral. It will bring some errors and we will discuss the problem in detail below.

Usually, \( N(k) \) can be written in terms of the dimensionless variable \( kR \) as

\[
N(k) = A(kR)^3 + B(kR)^2 + C(kR) + N_{res}^{(0)}(k),
\]

where \( R \) is the radius of the bag. The first, second and third terms of the right hand side of Eq.(2) refer to the contributions of the volume, surface and curvature, respectively, and \( N_{res}^{(0)}(k) \) refers to other contributions which are not proportional to \((kR)^3, (kR)^2 \) or \((kR)\). We will discuss the term \( N_{res}^{(0)}(k) \) in section 3 in detail. In general, the coefficients \( A, B \) and \( C \) are expected to be functions of \( m/k \), and their expressions are model dependent. For example, using the box renormalization of the wave function, Jaqam et al obtained [11]

\[
A = \frac{2}{9\pi}, B = \frac{-1}{4}, C = \frac{1}{4},
\]

In their approximation, \( A, B \) and \( C \) are all constants and do not depend on the momentum. Of course, this treatment seems to be too rough because the plane wave is not the real eigenmode of the spherical bag geometry. The exact eigenfunctions of the spherical bag model, as shown earlier, are the spherical Bessel functions.

Another approach which is better than the plane wave approximation is the multi-reflection theory (MRT) [12], [13]. According to MRT, the volume term \( A \) can be fixed using the known total number of states for an infinite system with very large \( R \),

\[
\lim_{R \to \infty} A = A_\infty = \frac{2g}{9\pi},
\]

where \( g \) is the total number of degeneracies. For example, \( g \) is the total number of spin and color degrees of freedom for a quark with flavor treated separately. The surface term \( B \) was approximately derived from MRT to be [12]

\[
B_{MRT} \left( \frac{m}{k} \right) = \frac{g}{2\pi} \left\{ \left[ 1 + \left( \frac{m}{k} \right)^2 \right] \tan^{-1} \left( \frac{k}{m} \right) - \frac{\pi}{2} \right\},
\]

where \( m \) is the mass of a quark. The curvature term \( C \) has not even been evaluated the present except for the two limiting cases: \( m \to 0 \) and \( m \to \infty \) according to MRT. Madsen proposed [14], [15] an arbitrary form for the curvature term \( C \) that simply connects the above mentioned limits, namely

\[
\tilde{C} \left( \frac{m}{k} \right) = \frac{g}{2\pi} \left\{ \frac{1}{3} + \left( \frac{k}{m} + \frac{m}{k} \right) \tan^{-1} \frac{k}{m} - \frac{\pi k}{2m} \right\},
\]

to study the strangelet. Of course, this is only an ansatz with two correct limits.

Since the spherical bag geometry is popular for finite nuclei or quark systems and the DOS plays a key role in calculations, it is of interest to study this problem by exact numerical calculations under such a geometry. Gilson and Jaffe [16] evaluated the microscopic total number of quark states \( N(k) \) numerically under the MIT bag boundary condition for a fixed
quark mass \( m = 150 \text{MeV} \). This is appropriate to the nonrelativistic limit \( m > k \). To our knowledge, the mass dependence of the DOS found by numerical calculation is still lacking. The purpose of this paper is to check the MRT, especially the surface term given by Eq.\( (5) \) and the curvature term by Eq.\( (6) \), and to find the mass dependence of the DOS by numerical counting of the eigenmode under the MIT bag boundary condition. This is of value because our knowledge of \( N(k) \) is improved through the following analysis:

1. A numerical study of the mass dependence of the surface term and the curvature term using a smooth representation which would best fit the total number of quark states obtained from the numerical data.
2. Comparison of the surface term to the MRT result to provide a first principle’s check of the theory.
3. Extraction of the unknown curvature term from the numerical data to provide a suitable smooth representation, instead of Eq.\( (6) \), our representation is not only correct at the two limits \( m \to 0 \) and \( m \to \infty \), but can also be used in the whole mass region.
4. Study of the extent to which the smooth representation of \( N(k) \) can be applied.

The organization of this paper is as follows: Section 2 contains a description of the procedure for numerical calculation of the total number of quark states. In section 3, the resulting fluctuating numerical data are fitted by using a smooth representation for the same quantity to obtain the coefficients of the volume, surface and curvature terms. The fluctuations and their behaviour under smoothing of the remaining part of the numerical data are also studied in this section. Section 4 is our conclusion, discussion and the results for the DOS using a non-relativistic boundary condition.

II. NUMERICAL EVALUATION

The quarks inside a MIT bag are free Dirac particles bouncing back and forth from the infinite barrier on the bag surface. Their discrete energies in a spherical bag are determined by the MIT boundary condition \[ (i\gamma^\mu \psi - \psi)|_{\partial V} = 0, \] where \( \psi \) is the wave function for quarks, \( \partial V \) the MIT bag surface and \( n^\mu \) the outward unit vector which is normal to the MIT bag surface in its rest frame. The eigenstates of the quarks in such a spherical cavity can be written as

\[
\psi_{n\kappa M} (\mathbf{r}) = \begin{pmatrix} \frac{u_{nk}(x)}{x} Y_{\kappa M}(\hat{r}) \\ i \frac{v_{nk}(x)}{x} Y_{-\kappa M}(\hat{r}) \end{pmatrix},
\]

with \( x = qr \) and \( q \) the absolute value of the 3-momentum of the quark. Here, \( \hat{r} \) is the unit vector pointing in the same direction as the coordinate vector \( \mathbf{r} \) for the quark. The sub-indices \( n = 0, 1, 2, \ldots \), \( \kappa = \pm 1, \pm 2, \ldots \), and \( M \) are quantum numbers besides the flavour and color that completely specify a single quantum state \[ ]\ for a quark. The radial wave

\[ \]
functions \( u_{n\kappa} \) and \( v_{n\kappa} \) are proportional to spherical Bessel functions since the quarks are free particles inside the bag. The spin-orbital angular momentum coupled wave functions, have a total angular momentum \( j = |\kappa| - 1/2 \) are \( Y_{\kappa m} \) and \( Y_{-\kappa m} \). The orbital angular momentum \( l \) for \( Y_{\kappa m} \) is \( j - 1/2 \) if \( \kappa < 0 \) and \( j + 1/2 \) if \( \kappa > 0 \). Imposing Eq.(7) on the wave function Eq.(8), we get

\[
u_{n\kappa}(qR) = v_{n\kappa}(qR), \tag{9}
\]
which can be numerically solved for each \( n \) and \( \kappa \) to get a discrete set of \( q_{n\kappa} \). The energy \( \epsilon \) for a quark in such a state is

\[
\epsilon_{n\kappa} = \sqrt{q_{n\kappa}^2 + m^2}. \tag{10}
\]

This has a one to one correspondence to \( q_{n\kappa} \). It is expected that the value for each \( \epsilon_{n\kappa} \) has to be obtained numerically for the MIT bag boundary condition.

The approach of summation over the microscopic energy levels to obtain the thermodynamical potential is rather computationally expensive. For example, the thermodynamical potential of a strangelet can be written as

\[
\Omega = -\frac{n_c}{\beta} \sum_{f=\{u,d,s\}} \sum_{n=0}^{\infty} \sum_{\kappa=-\infty}^{\infty} (2j_\kappa + 1) \ln \left( 1 + e^{-\beta(\epsilon_{f\kappa\mu_f})} \right) + \Omega', \tag{11}
\]

where \( \beta \) is the inverse temperature, the summation over \( \kappa \) excludes \( \kappa = 0 \), \( j_\kappa \) is the total angular momentum of the state corresponding to \( \kappa \), \( \mu_f \) is the chemical potential for flavor \( f \), \( n_c = 3 \) is the degeneracy due to the color degrees of freedom of quarks, and \( \Omega' \) is the contribution to the thermodynamical potential from other degrees of freedom of the system.

In most of the cases, the quantity being summed is a smooth enough function of the quark energy on the scale that the DOS fluctuates. To study the gross features, we can introduce the concept of DOS and replace the microscopic summation by an integration over the quark’s momentum, namely

\[
\sum_{\epsilon_{n\kappa}} F(\epsilon_{n\kappa}) \to \int_0^\infty dk \rho(k) F[\epsilon(k)]. \tag{12}
\]

Here \( \epsilon_{n\kappa} \) is the discrete energy level, \( \epsilon(k) \) is its continuous interpolation using Eq.(11), and \( \rho(k) \) is the DOS which is determined by the total number of quark states \( N(k) \). In the numerical calculation, the \( \overline{N}(k) \) that provides the best fit to \( N(k) \) is used as a smooth representation of \( N(k) \). With a smooth \( \overline{N}(k) \), the DOS \( \rho(k) \) in the above equation is then

\[
\rho(k) = \frac{d\overline{N}(k)}{dk}. \tag{13}
\]

There is no guarantee that the left hand side of Eq.(12) is the same as its right hand side in the case studied here, since the microscopic distribution of the energy levels does not follow a trend regular enough to avoid the fluctuations introduced by \( \overline{N}(k) \) replacing \( N(k) \). In fact, as is found in the following, the fluctuations in the DOS are large and irregular. However, the situation can be improved by expressing Eq.(12) as

\[
\sum_{\epsilon_{n\kappa}} F(\epsilon_{n\kappa}) \to \int_0^\infty \rho(k) F[\epsilon(k)].
\]
\[ \sum_{n} F(\epsilon_{n}) = \int_{0}^{\infty} dk \rho(k) F(\epsilon(k)) + <\delta F>, \]  

(14)

where \(<\delta F>\) is by definition the difference between the left and right hand side of Eq.(12). It is easy to see that \(<\delta F> = 0\) if

\[ <N - \overline{N}> (k) = \sum_{k_i} \left[ N(k_i) - \overline{N}(k_i) \right] \rightarrow 0, \]

(15)

where the summation is over the energy levels of quarks with a magnitude of 3-momentum in the neighborhood of \(k\) in which \(F[\epsilon(k)]\) does not change appreciably. The best we can do to find the general trend of the problem is to extract from \(N(k)\) as precisely as possible the smooth quantity \(\overline{N}(k)\) which can be attributed to the DOS. The quantity \(<\delta F>\) is then usually small and can be ignored.

The total quark states with the momentum \(q \leq k\) for each flavor is counted according to

\[ N(k) = n_c \sum_{n=0}^{\infty} \sum_{\kappa=-\infty}^{\infty} \theta(k - q_{n\kappa})(2j_{\kappa} + 1), \]

(16)

where \(q_{n\kappa}\) is determined by Eq.(11) and the step function \(\theta(x) = 1\) if \(x > 0\), and \(\theta(x) = 0\) if \(x < 0\). This number is, in principle, a function of three variables, namely, the cutoff momentum \(k\), the mass \(m\) and the bag radius \(R\). Since \(N(k)\) is a dimensionless number, it is expected to be a function of dimensionless variables too. Two such kinds of variables, namely, \(m/k\) and \(kR\) formed by \(k\), \(m\) and \(R\) have been chosen in Eq.(12) while the other variables, for example \(mR\), will not emerge in expressions of coefficients \(A\), \(B\) and \(C\) because they are independent of \(R\).

The numerically counted \(N(k)\) is therefore fitted by using the following smooth trial functional form ansatz

\[ \overline{N}(k) = A \left( \frac{m}{k} \right) (kR)^3 + B \left( \frac{m}{k} \right) (kR)^2 + C \left( \frac{m}{k} \right) (kR), \]

(17)

where all coefficients \(A\), \(B\) and \(C\) are assumed to be independent of \(kR\).

The detailed fitting is done in the following way, First, \(m\) and \(k\) are kept fixed (so \(m/k\) is a constant), and various corresponding \(N(k)\) are counted by varying \(R\). Such a series of \(N(k)\) data as a function of \(R\) is fitted using the smoothed representation Eq.(17) to obtain the coefficients \(A\), \(B\) and \(C\) for a fixed \(m/k\). We employ “the method of minimum squares” to obtain the best fit. Then the value of \(m\) is changed with a fixed \(k\) and the above steps are repeated to obtain a different \(A\), \(B\) and \(C\) for different \(m/k\).

The consistency of the procedure is checked by calculating \(N(k)\) with a series of different cutoff momentum \(k\) (25,50,100,200,400 and 800 MeV) with \(m/k\) and \(kR\) fixed. It is found that the choice of cutoff momentum will not affect the coefficients \(A(m/k)\), \(B(m/k)\) and \(C(m/k)\) for each \(m\) and \(k\) bin.

III. SMOOTHED PART OF THE DOS UNDER THE BAG BOUNDARY CONDITION

The results of our best fit for smooth curves by using “the method of minimum squares” can be summarized as follows.
A. The volume term

The volume term $A$ is found to be

$$A \left( \frac{m}{k} \right) = 7.074 \times 10^{-2} g,$$  \hspace{1cm} (18)

which is different from $2g/9\pi$ by a difference of $10^{-4} - 10^{-5}$. It means that $A(m/k)$ is independent of $m/k$ to a very good approximation. This result is in good agreement with the MRT as well as the plane wave approximation.

B. The surface term

The coefficient $B(m/k)$ depends on $m/k$ explicitly. The results of our best fitted $B(m/k)$ is compared to the one from the MRT. The relative difference between $B(m/k)$ and $B_{MRT}(m/k)$ is shown in Fig. 1. It can be seen that such a relative difference is around $1 - 2\%$ for most of the $m/k$ value except at rather small $m/k$. Thus we come to the conclusion that the coefficient $B_{MRT}(m/k)$ describes the surface correction of the DOS very well.

C. The curvature term

After we remove the volume term and the surface term, the remaining numerical data for $N(k)$, which is denoted as $N^{(1)}_{res}(k)$, contains information about the coefficient of the curvature term $C(m/k)$. The fluctuations of $N^{(1)}_{res}(k)$ are large. To extract the linear term, an average of the remaining data $N^{(1)}_{res}(k)$ defined by

$$N^{(1)}_{res}(kR) \approx \frac{1}{\Delta} \sum_{x=x=kR-n\delta x \Delta/2}^{kR+n\delta x \Delta/2} N^{(1)}_{res}(x),$$ \hspace{1cm} (19)

where $\delta x$ is the difference between the neighbouring $kR$ points in the numerical data for $N(k)$, is made first. The averaged $N^{(1)}_{res}$ is fitted to a linear function by using the method of minimum squares to get the curvature term. The resulting coefficient $C(m/k)$ is not a slow varying function of $m/k$ as is the one assumed in Eq.(6). The result of our best fit for $\Delta = 50$ is shown in Fig. 2 which agrees with the multi-reflection theory at the two ends, $m/k = 0$ and $m/k \rightarrow \infty$, but is a fluctuating function of $m/k$ in between. If these fluctuations are smoothed out, it contains a global maximum which is different from the proposed monotonic function given in Eq.(6). A smooth representation of the extracted (fluctuating) function is the following

$$C(m/k) = \tilde{C}(m/k) + \left( \frac{m}{k} \right)^{1.45} \frac{g}{3.42 \left( \frac{m}{k} - 6.5 \right)^2 + 100}$$ \hspace{1cm} (20)

with $\tilde{C}(m/k)$ given by Eq.(6). This is plotted as the solid line in Fig. 2 together with the numerical data points. The dashed line is $\tilde{C}(m/k)$.
D. Fluctuating term

Most of the fluctuations $N(k)$ reside in the remaining part of Eq.(2). It is also expected that the difference between the smoothing procedure of the MRT and the one adopted here resides in this residual term, which is obtained from the numerical data $N(k)$ using the following equation

$$N_{\text{res}}^{(0)} = N(k) - \frac{2g}{3\pi}(kR)^3 - B(m/k)(kR)^2 - C(m/k)(kR),$$

(21)

where $B(m/k)$ and $C(m/k)$ are obtained from the procedure above described. We use the method for $N_{\text{res}}^{(0)}$ of Eq. (19) to smooth $N_{\text{res}}^{(0)}$ and obtain $N_{\text{res}}^{(0)}(\Delta k)$.

The results for $\Delta = 1, 10, 50, 100$ and $m/k = 0.1, 100$ are shown in figure 3 and figure 4, respectively. Two trends for the numerical data are seen after subtracting the volume, surface and curvature terms obtained by best fitting. First the magnitude of the fluctuations decreases as $1/\sqrt{\Delta}$. Secondly, the magnitude of the fluctuations increases with $kR$. The fluctuations will exist for any value of $\Delta$.

This result means that $N_{\text{res}}^{(0)}$ can not in principle be treated as zero. According to Eq.(14), this means that the fluctuating term $<\delta F>$ for any smooth function of $k$ is not zero for the MIT bag model. Fortunately, it is not very large for a smooth function ($N_{\text{res}}^{(0)}/N \approx 10^{-5} \sim 10^{-6}$) and can be dropped in most of the applications involving the gross features of the problem.

IV. CONCLUSION AND DISCUSSION

The distribution of the quark states in a spherical MIT bag is calculated numerically. By making a best fit to the data using a smooth function of the dimensionless variables $kR$ and $m/k$, the coefficient of this kind of power expansion is determined. It is found that the volume and surface terms can be represented by a smooth function of the above mentioned variables in agreement with the MRT. The curvature term which contains fluctuations is extracted from the numerical data and represented by a smooth function, as given by Eq.(20). The fluctuations remain after smoothing, but can be ignored in most problems.

The same treatment can also be applied to the non-relativistic case: For simplicity we only give the final result here. The DOS for non-relativistic particles confined in a spherical cavity of radius $R$ with boundary condition

$$u_{\xi}(kR) = 0$$

(22)

can be found and the best smooth fit to the numerical result is

$$N(k) = \frac{2g}{3\pi}(kR)^3 - 0.1289g(kR)^2 + 1.0144g(kR) - 60.319g.$$  

(23)

A non-spherical bag is needed to represent a droplet at high angular momentum, which is expected to be produced in relatively large number in a high energy relativistic heavy ion collision. This is not studied in this work. A representation and numerical study of these deformed bags should be carried out in the future.
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V. FIGURE CAPTIONS

FIG.1. The difference of the coefficient $B$ as a smooth function of $m/k$ between the one best fitted to the numerical counted value and the one calculated analytically. Their difference draw in line is almost a constant with a variation less or equals to 1% of its own value.

FIG.2. The coefficient $C$ extracted from $N_{\text{res}}^{(1)\Delta}$. The solid line is a smooth representation of it. The dashed line represents $\tilde{C}(m/k)$.

FIG.3. The behaviour of the fluctuating residual term $N_{\text{res}}^{(0)}$ under the smoothing for $m/k = 0.1$.

FIG.4. The behaviour of the fluctuating residual term $N_{\text{res}}^{(0)}$ under the smoothing for $m/k = 100$. 
Figure 1

\[
\frac{(B-B_{MRT})}{B_{MRT}}
\]

\[
\times 10^{-2}
\]

[m/k]
Figure 2
Figure 3
Figure 4