On early onset of quark number density at zero temperature

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We study a longstanding problem in lattice QCD at low temperature and nonzero quark chemical potential on an onset of the quark number density at \( \mu = m_\pi/2 \). We introduce a physical parametrization of the eigenvalues in the reduction formula of the fermion determinant. It is shown that the parametrization reduces the quark number density operator to an expression with the Fermi distribution of the quark. For each configuration, the eigenvalues of the reduced matrix correspond to one-particle energy states of a quark. The gap of the eigenspectrum of the reduced matrix corresponds to the gap of the energy states, which causes the \( \mu \)-independence of the fermion determinant for small \( \mu \) at \( T = 0 \). Once \( \mu \) exceeds the gap, the quark number density becomes nonzero for each configuration, which causes the early onset of the quark number density.

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Properties of QCD at finite temperature (\( T \)) and quark chemical potential (\( \mu \)) are central issues in particle, nuclear and astrophysics in order to understand various states of matter in our universe. One important nature of QCD is the deconfinement transition. Recent simulations on finer lattices show that the deconfinement transition is crossover [1], and occurs at \( T_{\text{pc}} = 150 - 170 \text{ MeV} \) depending on observables [2,4]. It is expected that the crossover extends to nonzero \( \mu \) and turns into a first order phase transition at a critical endpoint(CEP), which has been studied in many references, e.g. [3,6].

The QCD phase diagram is expected to contain rich structures also at low temperatures [5,7,8]. In addition, the discovery of a pulsar with twice solar mass [9] calls the reliable recovery of a pulser with twice solar mass [9] is a significant event. The other one was to take the low temperature limit of \( \mu = \mu_c \) and turn into a first order phase transition at a critical endpoint(CEP), which has been studied in many references, e.g. [14,15], the solution is not yet obtained. In order to reveal the QCD phase diagram based on first principle lattice simulations, one must confront this problem.

It was shown theoretically [16,17] that the fermion determinant \( \det \Delta(\mu) \) is independent of \( \mu \) at \( T = 0 \). Cohen showed the \( \mu \)-independence for isospin chemical potential case by considering the \( \gamma_0 \) times the Dirac operator. Adams showed it for quark chemical potential case by using a reduction formula for the fermion determinant. For lattice QCD, we showed the \( \mu \)-independence of \( \det \Delta(\mu) \) by using the reduction formula [18] in two approaches. One approach was to evaluate the \( \mu \)- and \( T \)-dependence of a factor \( \det \Delta(\mu)/\det \Delta(0) \). We found that the factor becomes insensitive to \( \mu \) as \( T \) decreases. The other one was to take the low temperature limit of \( \det \Delta(\mu) \) with the aid of properties of the reduced matrix, a \( N_f \) scaling law, the existence of a gap, pair nature and a relation between the gap and pion mass. We found that those properties makes \( \det \Delta(\mu) \) \( \mu \)-independent for \( \mu < m_\pi/2 \).

Thus, the \( \mu \)-independence of the fermion determinant at low \( T \) and small \( \mu \) was explained both in theoretical studies and lattice simulations. It is likely that the approaches in Refs. [16-18] are closely related. Now, it is meaningful to consider underlying physics beyond the early onset of the quark number density by extending the previous approaches.

In this paper, we address the problem of the early onset of the quark number density by using the reduction formula. According to the previous studies, we introduce a physical parametrization of the eigenvalues of the reduced matrix \( Q \). It will be shown that the parametrization reduces the number density operator of the quark to an expression with the Fermi distribution. This makes it possible to study the property of the quark number density at \( T = 0 \) in a familiar technique. The gap of the eigenvalues of \( Q \) plays a similar role to a Fermi energy in the Fermi distribution. The \( \mu \)-independence of \( \det \Delta(\mu) \) at \( T = 0 \) is explained by a simple argument based on the Fermi distribution with the energy gap. We will discuss the origin of the early onset.

We employ clover-improved Wilson fermions of \( N_f = 2 \). The result can be applied to other actions if the reduction formula is available. First we divide the Wilson fermion matrix \( \Delta \) into the spatial part and temporal part,

\[
\Delta(\mu) = B - \kappa \begin{bmatrix} e^{+\mu a}(r - \gamma_i)U_4(x)\delta_{x',x+4} \\
+e^{-\mu a}(r + \gamma_i)U_4^\dagger(x')\delta_{x',x-4} \end{bmatrix},
\]

(1)

\[
B = \delta_{x,x'} - \kappa \sum_{i=1}^{3} \left[(r - \gamma_i)U_{i}(x)\delta_{x',x+i} + (r + \gamma_i)U_{i}^\dagger(x')\delta_{x',x-i} \right] - \kappa C_{SW} \delta_{x,x'} \sum_{\mu \leq \nu} \sigma_{\mu\nu} F_{\mu\nu},
\]

(2)

where \( B \) is the spatial Wilson matrix, \( \kappa \) the hopping parameter, \( r \) the Wilson parameter, \( C_{SW} \) the clover coefficient. We introduce two block-matrices

\[
\alpha_i = B^{ab,\mu\sigma}(\vec{x},\vec{y},t_i) r^{-\sigma\nu} - 2 \kappa r^\mu a \delta^{\mu\nu} \delta(\vec{x} - \vec{y}),
\]

(3a)

\[
\beta_i = \left[B^{ac,\mu\sigma}(\vec{x},\vec{y},t_i) r^{\sigma\nu} - 2 \kappa r^\mu a \delta(\vec{x} - \vec{y}) \right]U_4^{\dagger b}(\vec{y},t_i),
\]

(3b)
where $\xi = e^{-\mu/T}$, $N = 4N_cN_fN_t$ and $N_{\text{red}} = N/N_t$. $N$ and $N_{\text{red}}$ are the dimensions of $\Delta$ and $Q$, respectively. $Q$ and $C_0$ are independent of $\mu$. Calculating $|Q - \lambda I| = 0$, we obtain

$$\det \Delta(\mu) = C_0 \xi^{-N_{\text{red}}/2} \prod_{n=1}^{N_{\text{red}}} (\lambda_n + \xi),$$

with a fixed scale $\alpha$. The agreement of the results indicates that an eigenvalue is parametrized as $|\lambda| \sim l^{N_t}$, where $l$ is a real. In Ref. [18], we derived the low-$T$ limit of $\det \Delta(\mu)$ by using these properties of $\lambda$, and found that $\det \Delta(\mu)$ is $\mu$-independent for $\mu < m_{\pi}/2$ in the low $T$ limit.

According to the $N_t$ scaling law, we introduce a parametrization of the eigenvalues of $Q$ as $|\lambda| = \exp(-e/T)$ and $|1/\lambda^*| = \exp(e/T)$, where we describe larger half of the eigenvalues in terms of the smaller half of the eigenvalues. This parametrization was also implied in Ref. [17] and suggested from an analogy between $Q$ and the Polyakov line [18]. The Polyakov loop describes the free energy of static quarks in heavy quark limit: $\langle P \rangle \sim e^{-F/T}$ with $P = \text{tr} \prod_{i=1}^{N_t} U_4(t_i)$. Considering an eigenvalue $\lambda$, $|\lambda| < 1$, the analogy between $P$ and $Q$ may suggest that $\lambda$ is related to an energy of a dynamical quark. The eigenvalue $1/\lambda^*$ has the counterpart $1/\lambda^*$. Because the pair nature results from the $\gamma_5$ hermiticity, it is natural to identify $1/\lambda^*$ as an energy of an anti-quark.

Adams showed that the reduction formula reproduces the fermion determinant obtained from a Matsubara frequency summation method in free field case [17]. We show this correspondence in the present case. Using the pair nature of the eigenvalues, Eq. (5) can be rewritten as

$$\det \Delta(\mu) = C_0 \prod_{n=1}^{N_{\text{red}}/2} (\lambda_n^* e^{\xi})^{-1}(1 + \lambda_n e^{-\xi})(1 + \lambda_n^* e^{\xi}).$$

For a while, we drop the phase of $\lambda$. If we substitute $\lambda = e^{-\xi/T}$ and $\xi = e^{-\mu/T}$, then Eq. (6) is reduced to

$$\det \Delta(\mu) = C_0 \prod_{n=1}^{N_{\text{red}}/2} e^{\xi/T}(1 + e^{-e(-\mu)/T})(1 + e^{e(-\mu)/T}),$$

which agrees with the Matsubara frequency summation method. Note that there is a degeneracy of Dirac components in the free field case. This correspondence suggests that

$${r}_\pm = (r \pm \gamma_4)/2$$ are projection operators in case of $r = 1$, which is used in the derivation of the formula. Using the block matrices, $\det \Delta(\mu)$ is given by

$$\det \Delta(\mu) = \xi^{-N_{\text{red}}/2} C_0 \det (\xi + Q),$$

$Q = \prod_{i=1}^{N_t}(\alpha_i^{-1} \beta_i)$, $C_0 = \prod_{i=1}^{N_t} \det(\alpha_i)$, which is used in the derivation of the formula.

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\( \epsilon a = - \ln |\lambda|/N_t \) describes one-particle energy states of a quark for a single configuration.

Here, we comment on the ensemble average. The reduction formula provides the fugacity expansion of the fermion determinant: \( \det \Delta (\mu) = \sum c_n e^{\mu \lambda_n} \), where \( c_n \) are functions of \( \lambda_n \). Taking ensemble average correctly, a canonical partition function with a fixed quark number can be obtained, which provides a physical free energy of QCD. On the other hand, \( \epsilon \) corresponds to one-particle energy states of a quark for single configuration. This is perhaps related to a “quasi-energy” introduced in Ref. [16], which is eigenvalues of the Dirac operator. The ensemble average is crucial to calculate thermodynamical quantities, while it is convinient to consider \( \epsilon \) for the present purpose.

Let us consider the number density operator. Equation (6) is rewritten as

\[
\det \Delta (\mu) = C_0 \exp \left( \sum_{n=1}^{N_{\text{ud}}} \left[ - \ln \lambda_n^* + \ln (1 + \lambda_n \xi^{-1}) + \ln (1 + \lambda_n^* \xi) \right] \right). \tag{8}
\]

For large volume, it is reduced to a spectral representation

\[
\det \Delta (\mu) = C_0 \exp \left( 4 N_c V_s \int_{|\lambda| < 1} d\lambda \rho(\lambda) \left[ - \ln \lambda^* + \ln (1 + \lambda \xi^{-1}) + \ln (1 + \lambda^* \xi) \right] \right). \tag{9}
\]

Here \( V_s = N^3_c \), and \( \rho(\lambda) \) is the spectral density defined on the complex \( \lambda \) plane. \( \rho \) is normalized by

\[
\int d\lambda \rho(\lambda) = 1, \tag{10a}
\]

\[
\int_{|\lambda| \leq 1} d\lambda \rho(\lambda) = \int_{|\lambda| \geq 1} d\lambda \rho(\lambda) = \frac{1}{2}. \tag{10b}
\]

Here the normalization conditions are satisfied in any \( N_t \).

The number density operator for quarks is given by \( \hat{n} = [V_s^{-1} T (\partial/\partial \mu) \det \Delta (\mu)] / \det \Delta (\mu) \). We obtain

\[
\hat{n} = \int_{|\lambda| < 1} d\lambda \rho(\lambda) \left( \frac{\lambda \xi^{-1}}{1 + \lambda \xi^{-1}} - \frac{\lambda^* \xi}{1 + \lambda^* \xi} \right). \tag{11}
\]

Now, we employ \( \lambda = e^{-\epsilon/T + i\theta} \) and \( \xi = e^{-\mu/T} \),

\[
\hat{n} = \int_{|\lambda| < 1} d\lambda \rho(\lambda) \left( \frac{1}{1 + e^{(\epsilon-\mu)/T-i\theta}} - \frac{1}{1 + e^{(\epsilon+\mu)/T+i\theta}} \right), \tag{12}
\]

and

\[
\int_{|\lambda| < 1} d\lambda = \int_0^\infty \frac{d\epsilon}{T} e^{-2\epsilon/T} \int_{-\pi}^{\pi} d\theta. \tag{13a}
\]

Then,

\[
\hat{n} = \int_0^\infty \frac{d\epsilon}{T} e^{-2\epsilon/T} \int_{-\pi}^{\pi} d\theta \rho(e^{-\epsilon/T+i\theta}) \times \left( \frac{1}{1 + e^{(\epsilon-\mu)/T-i\theta}} - \frac{1}{1 + e^{(\epsilon+\mu)/T+i\theta}} \right), \tag{14}
\]

where aside from \( \theta \), the first term in the large bracket is the Fermi distribution for a quark and the second term is that for an anti-quark.

Once having the Fermi distribution, the zero temperature limit is obtained from a familiar technique. Taking \( N_t \to \infty \) with a fixed lattice spacing \( a \), the Fermi distribution is reduced to the step function. It is obvious from \( N_t \)-independence of Eq. (10) that the factor \( e^{-2\epsilon/T}/T \) does not cause any ill-behavior in \( N_t \to \infty \). Then, we obtain

\[
\hat{n} = \int_0^\mu \frac{d\epsilon}{T} e^{-2\epsilon/T} \int_{-\pi}^{\pi} d\theta \rho(e^{-\epsilon/T+i\theta}), \tag{15}
\]

where \( \mu \) corresponds to a Fermi energy, and energy states below \( \mu \) are occupied at \( T = 0 \).

The gap in the eigenspectrum of \( Q \) generates the minimum value \( \epsilon_{\text{min}} \) given by \( \max |\lambda| < 1 |\lambda| = \exp(-\epsilon_{\text{min}}/T) \). The average of \( \epsilon_{\text{min}} \) is shown in Fig. 2. No eigenvalue exists for \( \epsilon < \epsilon_{\text{min}} \). Hence, we obtain

\[
\hat{n}(\mu) = 0 \quad \text{for} \quad \mu < \epsilon_{\text{min}}. \tag{16}
\]

Thus, the quark number density is zero at \( T = 0 \) for small \( \mu \) for any configurations. According to Gibbs [20], \( \epsilon_{\text{min}} \) corresponds to half the pion mass \( \epsilon_{\text{min}}a = m_\pi a/2 \) for each configuration. An alternative expression was found in Ref. [21], where the expression was given for the ensemble average. Although there is a difference between the results in Ref. [20] and [21], it is expected [21] that the results become the same for large temporal lattice size. Hence, we employ \( \epsilon_{\text{min}} = m_\pi/2 \). \( \hat{n} \) is zero for configuration by configuration for \( \mu < \epsilon_{\text{min}} \), and therefore its average is also zero, \( \langle \hat{n} \rangle = 0 \).

Now, we discuss the onset of the quark number density. A phenomenological expectation is that the quark number density starts to differ from zero at \( \mu = M_N/3 \). This expectation is based on the fact that quarks are confined inside hadrons. The present result, e.g. Eq. (14) indicates that the introduction of the quark chemical potential actually affects an excitation of quarks even in the confinement phase at least for single configuration. For \( \mu < \epsilon_{\text{min}} \), \( \mu \) is not enough to excite quarks for any configurations, and the quark number density is zero. Once \( \mu \) exceeds \( \epsilon_{\text{min}} \), the chemical potential causes excitation of quarks and leads to nonzero quark number density for each configuration. This is the origin of the early onset of the quark number density.

However, it does not necessarily mean that the average of the quark number density is nonzero. Once \( \hat{n} \) takes nonzero
values, the phase of $\hat{n}$ also becomes nonzero. It is known that the sign problem becomes severe if $\mu$ goes beyond $\frac{m_\pi}{2}$ \[18\]. Hence, it is unclear what happens for $\frac{m_\pi}{2} < \mu < M_N/3$. The complex phase of $\hat{n}$ causes the cancellation of the quark number density over configurations, which may lead to $\langle \hat{n} \rangle = 0$ for $\mu < M_N/3$.

Another possibility is that finite density effects change $\epsilon_{\text{min}}$. The relation $\epsilon_{\text{min}} = \frac{m_\pi}{2}$ is based on the fact that the pion is the lightest hadron. Although QCD inequalities do not hold for finite density region, the pion is the lightest hadron at least for nuclear matter density. Hence the relation would hold at least for nuclear matter density. It seems that this possibility is unlikely. If $\langle \hat{n} \rangle = 0$ for $\frac{m_\pi}{2} < \mu < M_N/3$, then it would be a consequence of the cancellation of the quark number density over configurations.

In summary, we have addressed the longstanding problem of the onset of the quark number density. Based on previous studies, we considered it by using the properties of the reduction formula obtained from the lattice QCD simulations. We parametrized the eigenvalues of the reduction formula based on some properties of the eigenvalues. The parametrization reduces the quark number density operator to the form with the Fermi distribution of a quark, where the eigenvalues of the reduced matrix correspond to one-particle energy states of a quark at single configuration level. Then, the $\mu$-independence of the fermion determinant is explained by the familiar technique. The present result shows that the quark chemical potential actually affects an excitation of quarks. Small $\mu$ can not excite any quark at $T = 0$, which causes the $\mu$-independence of the fermion determinant at $T = 0$. On the other hand, if $\mu$ exceeds a certain value related to the pion mass, it can excite quarks even in the confinement phase at least one-configuration level, which is the origin of the early onset of the quark number density. If the quark number density remains zero up to $\mu = M_N/3$, the complex phase of the quark number density would cause the cancellation over configurations. This result provides a hint to go beyond $\mu = \frac{m_\pi}{2}$ in lattice simulations.

For further confirmation, the spectral properties of the reduced matrix should be investigated in future lattice simulations for smaller quark mass, and larger lattice. Particularly, the behavior of the gap and $N_t$-dependence are important. It is also important to study the onset of the baryon number density by both theoretical and experimental studies. Our result suggests the validity of the phase quench QCD and the orbifold equivalence at low temperature for $\mu < \frac{m_\pi}{2}$ \[22\]\[23\]. Phase quench simulations are also interesting for small $\mu$.

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