Chiral symmetry breaking, instantons, and monopoles in lattice QCD by Supercomputer SX

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1 Introduction

Recently, some significant results have been reported by a research group [1, 2]. They claim that they create magnetic monopoles and observe them in a condensed matter system. They have discovered an evidence that the magnetic monopoles can exist in the real nature for the first time, since Paul A. M. Dirac predicted the magnetic monopole in the quantum theory in 1931 [3]. Furthermore, an interesting experiment at the Large Hadron Collider (LHC) was approved in 2010. The name of the experiment is the Monopole and Exotics Detector at the LHC (MoEDAL) experiment. One purpose of the experiment is to search "the massive magnetically charged particles as the magnetic monopole or the dyon[1]".

Also in the strong interaction physics of Quantum chromodynamics (QCD), the monopole has been considered, where it is expected to play a unique role in explaining the mechanism of color confinement. As explained in detail below, the condensation of monopoles may explain the confinement of the color flux just as the dual version of the ordinary superconductor where the electric charge of the Cooper pair condensates and magnetic flux is excluded. Our purpose of this research is to examine the interactions between monopoles, quarks, and gluons. We add monopoles by the monopole creation operator to the vacuum of QCD [4], and compute the observable quantities in experiments, using the supercomputer SX-ACE [Fig. 1]. This is primarily to clarify the mechanism of color confinement of QCD. In the future, we would like to further extend our research to the observation of monopoles and the evaluation of monopole effects in the NICA.

Figure 1: The supercomputer SX-ACE[2].

Quarks are the fundamental particles that interact by the strong force in the elementary particle physics. The gluons mediate the strong interaction between quarks. The strong force becomes weak in the high energy (short distance) region, and becomes strong in the low energy (long distance) region. This property of the strong force is called the asymptotic freedom (and infrared slavery), and is the important feature of QCD. In the high energy region, theoretical predictions by perturbative calculations reproduces nicely many experimental results. In the low energy region, however, we can not perform perturbative calculations. Therefore, methods of non-perturbative calculations are needed, which can be performed numerically by the first principle calculation using the supercomputers. That is the Lattice QCD. To study QCD in the low energy region, the supercomputer is one of the most important tools.

The low energy dynamics of the strongly interacting matter is also the issue of experimental studies. As one of recent projects, we would like to note a new Nuclotron-based Ion Collider fAcility (NICA) for the investigation of the phase structures of the quark matter at the Joint Institute for Nuclear Research (JINR, Dubna, Russia)[3]. The experiment is scheduled to start in 2018. The aim of the experiment is to study the hot and dense nuclear matter, the phase transition of the quark-gluon plasma

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[1] http://moedal.web.cern.ch/content/moedal-physics-programme
[2] The photo is taken from the NEC web page:
\http://jpn.nec.com/hpc/sxace/
[3] http://nica.jinr.ru/

(QGP), and the restoration of the chiral symmetry at the high baryon densities in heavy-ion collisions. These phenomenological issue are expected to be eventually related to the problems that we discuss in this report.

In the modern physics, the quark confinement is one of the biggest unsolved problems. An isolated quark has never been observed in experiments. The reason why the quarks are confined in mesons and baryons and can not be isolated, has not been shown yet. However, an important idea has been proposed by 't Hooft and Mandelstam. They explained the mechanism of the quark confinement in the maximal Abelian gauge in a beautiful manner [5, 6]. However, the Abelian monopole in the maximal Abelian gauge is the gauge-dependent quantity. Thus several attempts for the gauge-independent monopoles have been worked out in quenched SU(2) [7, 8]. The definition of the gauge-independent monopole has been also studied [9, 10].

In QCD, monopoles are non-perturbative object of the gluon field. It is know also that there is another non-perturbative object which is called the instanton. It is the non-trivial solution in the four-dimensional space-time, while the monopole is the three-dimensional one. The physics of instants is primarily related to spontaneous breaking of chiral symmetry [11, 12]. Because both monopoles and instantons are non-trivial objects of the gluon field of QCD, their relations have been discussed, though the detailed relations is not yet clear.

In our research, we focus on monopoles in QCD. We add the Abelian monopole and anti-monopole in the SU(3) non-Abelian gauge theory to the QCD vacuum by the monopole creation operator [4]. The monopole and the creation operator are studied by the Pisa group [4, 13, 14]. The Overlap fermion preserves the chiral symmetry in the lattice gauge theory [15, 16, 17]. Therefore, we examine the relation between the added monopoles and instantons in the QCD vacuum using the Overlap fermion as a probe, and show the relations between the monopoles and the chiral symmetry breaking.

We have already confirmed that the additional monopoles and anti-monopoles become the coherent state, and form the long loops in the QCD vacuum. We have quantitatively demonstrated that the additional monopoles and anti-monopoles create the instantons by comparing numerical results with analytical predictions [18]. We have shown that the chiral condensate (defined as a minus value) that is an order parameter for the spontaneous breakdown of the chiral symmetry, decreases by increasing the values of the monopole charges [19]. Moreover, the preliminary results have shown that the quark masses become slightly heavy by increasing of the values of the monopole charges [20]. These results suggest a dynamics of the QCD vacuum; that is, the additional monopoles and anti-monopoles become the coherent state in the QCD vacuum, furthermore, the monopoles create instantons and may induce the chiral symmetry breaking.

In a recent study, we check the effects of the finite lattice volume and the discretization on these results, using QCD vacuums of larger lattice volumes and the different parameters of the lattice spacing. Finally, we want to reveal the dynamics that monopoles would induce the chiral symmetry breaking, using the supercomputer SX.

In this article, we show an outline of achieved results in 2015 by the supercomputer SX-series.

2 Supercomputer SX-series

We have carried out numerical simulations since 2012, using the supercomputer SX-series at the Research Center for Nuclear Physics (RCNP) and the Cybermedia Center (CMC) at the University of Osaka in Japan.

Table 1: The number of cores N_{core}, computing performance (Perf.), and memory size (Mem.) per node. N_{node} indicates the number of nodes at CMC[5].

Series	N_{core}/node	Perf./node [GFLOPS]	Mem./node [GB]	N_{node}
SX-8R	8	256 - 282	64 - 256	20
SX-9	16	1600	1000	10
SX-ACE	4	276	64	1536

The supercomputer SX-series is produced by the NEC corporation (Japan), and possesses the "vector processors (array processors)". The Earth Simulator at the Japan Agency for Marine-Earth Science and Technology is one of the largest vector supercomputer systems in Japan. The vector supercomputers composed of the SX-ACE are highly parallelized, and used for the researches about the climate change and the earthquake[6].

The supercomputer SX-ACE has been used at the CMC since 2014. The information of the computing performance and memory size per node of the supercomputer SX-series at CMC are given in Table 1. The features of the SX-series are as follows:

- One node has a large shared memory.
- The computational speed is fast without making specially optimized parallel programs.
- The compiler of the SUPER-UX system automatically transforms original programs into highly optimized programs.

[5] http://www.hpc.cmc.osaka-u.ac.jp/en/category/system_intro-en/

[6] http://www.jamstec.go.jp/es/en/index.html

Table 3: Comparisons of the computational time (CPU time) for the Hermitian Wilson Dirac operator T_{Wi}, the Overlap Dirac operator T_{Ov}, and the total of the computational time T_{total}. The values are average values computed from the numbers of samples N_{conf}. The vectorization ratio of the computer programs for the SX-series is 99.9%.

V	Computer	N_{core}	Mem. [GB]	T_{Wi} [h]	T_{Ov} [h]	T_{total} [h]	N_{eigen}	N_{conf}
16^4	PC cluster	1	3.5	67(5)	112(5)	186(5)	80	10
	SX-8R	1	13.6	2.5(2)	18.8(5)	21.5(5)	80	10
	SX-9	1	13.7	1.78(12)	8.5(3)	10.5(3)	80	10
	SX-ACE	1	9.9	0.86(7)	6.7(4)	7.6(4)	80	5
18^4	SX-8R	1	20.9	1.89(15)	23(2)	25(2)	80	10
	SX-9	1	20.1	1.01(5)	9.0(3)	10.2(3)	80	10
	SX-ACE	1	15.7	0.74(16)	7.3(4)	8.2(5)	80	5

Table 2: The computational time (real time) $T_{comp.}$ for eigenvalue problems. The values are mean values computed from the numbers of configurations (statistical samples) N_{conf}. V indicates the lattice volume. N_{core} stands for the number of cores. N_{eigen} stands for the numbers of eigenvalues and eigenvectors in each configuration.

V	Computer	N_{core}	$T_{comp.}$ [h]	N_{eigen}	N_{conf}
16^4	SX-8R	1	19.8(6)	80	10
		4	13.6(6)	80	10
	SX-ACE	1	7.8(4)	80	5
		4	4.5(2)	80	5
18^4	SX-8R	1	22.1(5)	80	10
		4	11.3(4)	80	10
	SX-ACE	1	8.4(4)	80	7
		4	3.9(2)	80	5

We optimize computer programs for the supercomputer SX. The vectorization ratios of the computer programs are 99.7% $\sim$ 99.9%. The comparisons of the computational time for the eigenvalue problems used one or four cores of the SX-8R or the SX-ACE are given in Table 2. The computational time of the SX-ACE becomes about one-third comparing with the SX-8R.

3 The Dirac operators

The chiral symmetry refers to the invariance of Lagrangian by the chiral transformation. In the lattice gauge theory, the Dirac operator satisfying the Ginsparg-Wilson relation preserves the chiral symmetry. That is the massless Dirac operator D_{Ov} of the Overlap fermion. The Overlap fermion is the formulation of quarks in the lattice gauge theory, that preserves the chiral symmetry. The massless Overlap Dirac operator is composed of the Hermitian Wilson Dirac operator H_{Wi}. These operators are defined in Refs. [15, 16, 17, 21].

First, we generate the QCD vacuum in the quenched SU(3) by the standard Monte Carlo method, and compute the eigenvalues and eigenvectors from the QCD vacuum by solving the eigenvalue problems of the operators H_{Wi} and D_{Ov} (D) as follows:

$$D \mid \psi\rangle = \lambda \mid \psi\rangle \tag{1}$$

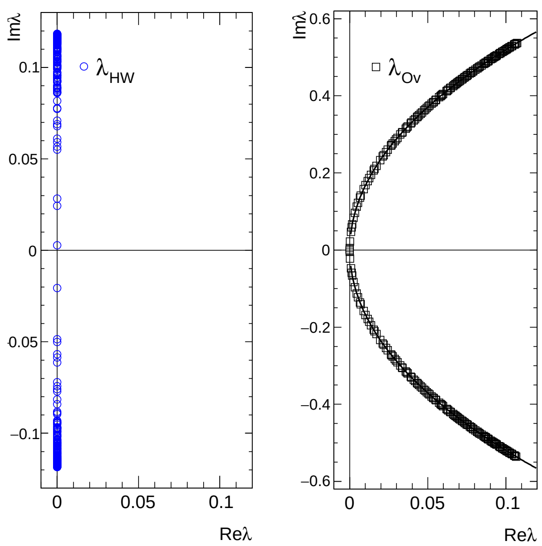

Figure 2: The spectra of the eigenvalues of the Hermitian Wilson Dirac operator λ_{HW} (left panel) and the Overlap Dirac operator λ_{Ov} (right panel). The number of eigenvalues N_{eigen} is 250. The eigenvalues are computed from one configuration. There is one zero mode in the spectrum of λ_{Ov}.

The eigenvalues of the Hermitian Wilson Dirac operator λ_{HW} are on the pure imaginary axis, whereas the pairs of eigenvalues of the massless Overlap Dirac operator $\pm\lambda_{Ov}$ are distributed on the circle centered at (1.4,

0) on the complex plane as shown in Fig. 2. The fermion zero modes can be found in the spectra of the eigenvalues of the massless Overlap Dirac operator, and the zero modes are fundamentally related to the chiral symmetry and spontaneous breakdown of the symmetry [21, 22].

To solve the eigenvalue problems, the optimized subroutines of ARPACK for the supercomputer SX in the mathematical library (MathKeisan) are used, and pairs of the eigenvalues and eigenvectors of the massless Overlap Dirac operator are saved. We used about 360,000 node hours for the computational time in 2015, and save about 100 terabytes in data storage areas. Almost all computational times are spent to find solutions of the eigenvalue problems of the massless Overlap Dirac operator.

The comparisons of the computational time for the Dirac operators H_{Wi} and D_{Ov} are given in Table 3. The total of the computational time T_{total} of the SX-ACE is about $\frac{1}{25}$ comparing with the PC cluster at the RCNP.

4 Instantons

The Atiyah-Singer index theorem suggests that the number of instantons can be computed from the number of fermion zero modes. However, we never simultaneously observed zero modes of the plus chirality n_+ and the minus chirality n_- from the same QCD vacuum. We assume that the physical lattice volumes of our system are too small to detect separately the plus or minus chiralities of the zero modes. Similar results are reported in Ref. [23]. We suppose that the observed zero modes N_{obs} are topological charges $Q = n_+ - n_-$, and the number of instantons N_i in our system is computed as follows:

$$N_i = \langle Q^2 \rangle = \langle N_{obs}^2 \rangle \qquad (2)$$

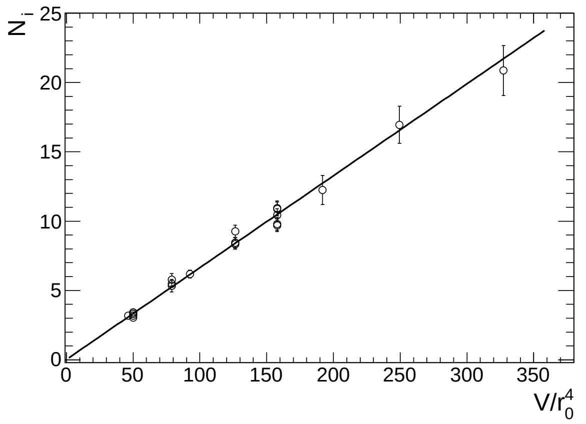

Figure 3: The number of instantons N_i ($\langle Q^2 \rangle$) vs. the physical volume V/r_0^4.

In order to show whether our supposition is correct, we fit a linear function $N_i = A \cdot V/r_0^4 + B$ to twenty-two points as shown in Fig. 3, and evaluate the instantons density ρ_i from the slope A. The fitted results are $A = 6.62(15) \times 10^{-2}$, $B = 2(10) \times 10^{-2}$, $\chi^2/n.o.f. = 20.4/20.0$. The intersect B is 0, and $\chi^2/n.o.f.$ is 1.0. That is, as the instanton liquid model predicts, the number of instantons is in direct proportion to the physical volume. The instanton density is

$$\rho_i = 8.04(18) \times 10^{-4} \text{ [GeV}^{-4}], \ (r_0 = 0.5 \text{ [fm]}). \qquad (3)$$

This value is exactly consistent with the prediction of the instanton liquid model [11]. These results denote that the number of instantons in the QCD vacuum is properly computed.

5 Instantons and monopoles

In this study, we create the Abelian monopoles in the SU(3) non-Abelian gauge theory by using the monopole creation operator [4]. The monopole fields are described in the Wu-Yang form [24]. The disorder parameter for the dual superconductivity of the QCD vacuum is defined from the monopole creation operator. The definition of the monopole, and the technique to create monopoles in the QCD vacuum has been studied by the Pisa group [4, 13, 14].

We generate QCD vacuums adding one pair of a monopole and an anti-monopole, varying the magnetic charges m_c by the monopole creation operator. The monopole has the positive magnetic charges and the anti-monopole has the negative magnetic charges. The total of magnetic charges is set to be zero. The magnetic charge m_c indicates that both the monopole of plus charges $+m_c$ and the anti-monopole of minus charges $-m_c$ are added. The magnetic charge $m_c = 0$ represents that monopoles are not added; the numerical results of $m_c = 0$ should be consistent with numerical results of the normal QCD vacuum. The details of the monopole creation operator and the monopoles are explained in Ref. [18].

First, in the maximal Abelian gauge we have confirmed that the monopole density increases and the length of monopole loops becomes longer by increasing the values of magnetic charges m_c. That is, the condensation of monopoles and anti-monopoles becomes the coherent state in the QCD vacuum.

Next, we solve eigenvalue problems of the massless Overlap Dirac operator, and compute the number of instantons from the number of fermion zero modes. In calculations, we do not perform the processes of smearing, cooling, or gauge fixing to the QCD vacuum. We find the quantitative relation between the number of monopole charges m_c and the number of instantons N_i by comparing with our prediction. We can not observe the zero modes

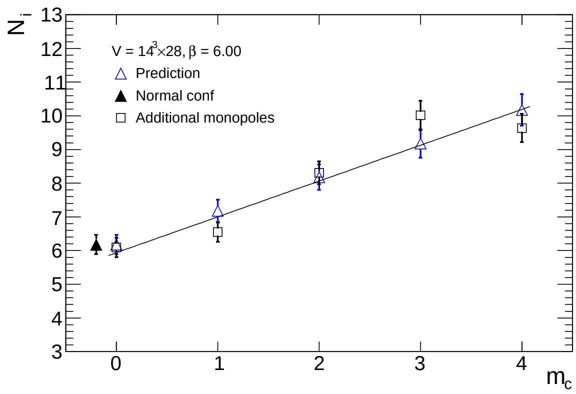

Figure 4: The number of instantons N_i ($\langle Q^2 \rangle$) vs. the value of the monopole charges m_c.

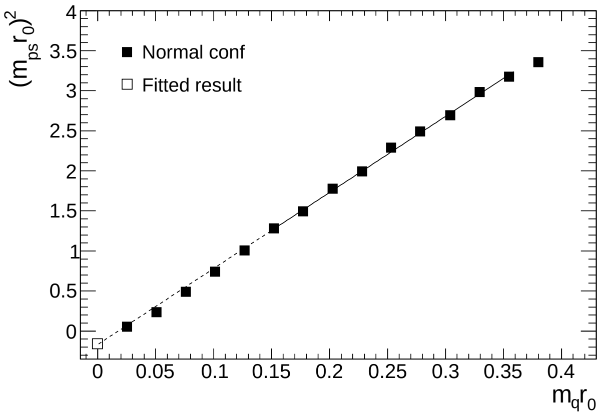

Figure 5: The square of the pseudo-scalar mass $(m_{ps}r_0)^2$ vs. the (valence) quark mass $m_q r_0$. The lattice is $V = 14^3 \times 28,\ \beta = 6.00$.

of n_+ and n_- in the same QCD vacuum, therefore, we make a hypothesis; one monopole of $+1$ magnetic charge and one anti-monopole of -1 magnetic charge would create one instanton of $+1$ or -1 charge. The instantons of positive charges and negative charges would be equally created for the CP invariance.

To confirm the hypothesis, we compare results that are computed from the analytical prediction with numerical results, by fitting a linear function $N_i = A \cdot m_c + B$ as shown in Fig. 4. If the slope A would be one, numerical results are consistent with our hypothesis. The fitted results are $A = 1.06(11),\ B = 5.9(2),\ \chi^2 = 9.1/3.0$. The value of the slope A is consistent with our hypothesis; one monopole of $+1$ magnetic charge and one anti-monopole of -1 magnetic charge create one instanton of $+1$ or -1 charge.

6 Chiral symmetry breaking and monopoles

A large number of theoretical and numerical results show that the monopole condensation is responsible for the quark confinement. Nevertheless, the relation between monopoles and the chiral symmetry breaking has not been clear yet, because the most common formulation of quarks (Wilson fermions) in the lattice gauge theory does not preserve the chiral symmetry.

In order to explain quantitatively the relation between the monopoles and the breakdown of the chiral symmetry, first, we evaluate the chiral (quark) condensate $\langle \bar{\psi}\psi \rangle$ numerically from the eigenvalues of the massless Overlap Dirac operator [25, 26, 27]. The chiral condensate is the order parameter for the chiral symmetry and the spontaneous breakdown of the symmetry.

- If the chiral symmetry is unbroken, the chiral condensate is zero.

$$\langle \bar{\psi}\psi \rangle = 0 \tag{4}$$

- If the chiral symmetry is spontaneous breakdown, the chiral condensate is not zero.

$$\langle \bar{\psi}\psi \rangle \neq 0 \tag{5}$$

  The quark obtains the mass through $\langle \bar{\psi}\psi \rangle$. The massless Nambu-Goldstone (NG) particle appears through the Axial-scalar channel $\pi \sim \bar{\psi} i \gamma_5 \psi$ [22].

First, we check the simple relation between the square of the pseudo-scalar mass m_π^2 and the quark mass m_q as shown Fig. 5. The pseudo-scalar mass m_π is computed from the eigenvalues and eigenvectors of the Overlap Dirac operator. The range of the physical quark mass is 10 [MeV] $\leq m_q \leq$ 150 [MeV], ($r_0 = 0.5$ [fm]). The fitted results are $A = 9.49(13)$, $B = -0.17(3)$, $\chi^2/n.o.f. = 7.4/7.0$, FR ($m_q r_0$ unit) : $0.15 - 0.36$. The intercept B does not become zero actually, but it is a comparatively small value.

In this study the chiral condensate is evaluated from the scale parameter Σ in the random matrix theory. In the epsilon-regime of QCD, the random matrix theory predicts universally the distributions of eigenvalues of the Dirac operators [28, 29]. We evaluate the chiral condensate by comparing the distributions of eigenvalues. The result of the chiral condensate at the continuum limit, considering the renormalization constant is [19, 27]

$$\langle \bar{\psi}\psi \rangle^{\overline{MS}}\ (2\ \text{GeV}) = -2.31(11) \times 10^{-2}\ [\text{GeV}^3] \tag{6}$$

$$= -\{285(4)\ [\text{MeV}]\}^3. \tag{7}$$

The value of the chiral condensate is not zero, and the pseudo-scalar mass m_π^2 becomes (about) zero at the limit

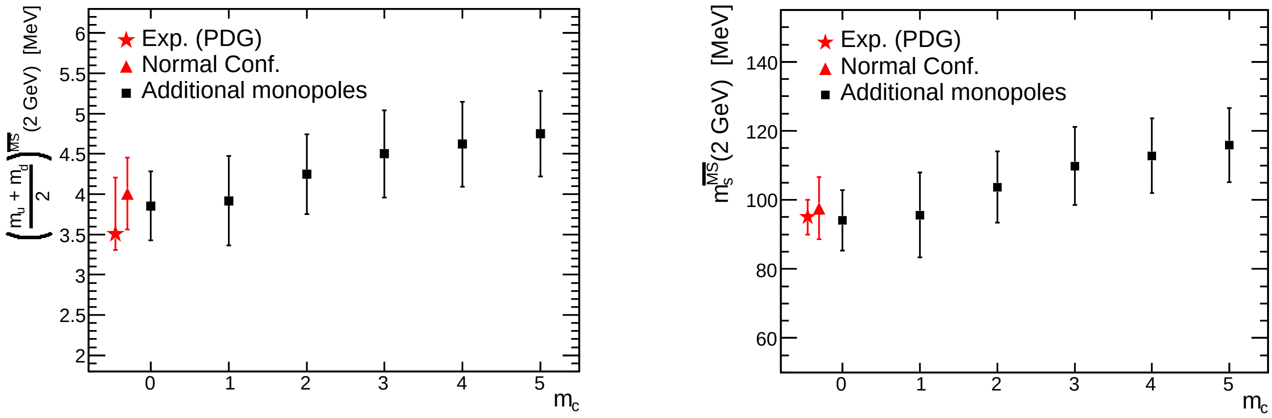

Figure 7: The quark masses in $\overline{\mathrm{MS}}$-scheme at 2 [GeV]; $\frac{m_u+m_d}{2}$ (left panel) and m_s (right panel) vs. the monopole charges m_c [20]. The lattice is $V = 16^3 \times 32$, $\beta = 6.00$.

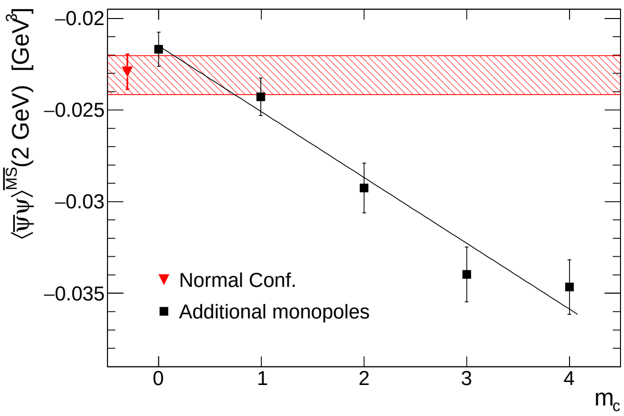

Figure 6: The chiral condensate vs. the monopole charges m_c [19]. The range enclosed by red lines indicates the result of the chiral condensate at the continuum limit (6).

$m_q \to 0$. These results are consistent with the Ward-Takahashi identity derived from the Ginsparg-Wilson relation [21]. That is to say, the Overlap fermion holds the chiral symmetry.

We have confirmed that the additional monopoles do not affect the spectra of the low-lying eigenvalues computed from the Overlap Dirac operator, and found that the additional monopoles change only the scale parameter Σ in the random matrix theory. Therefore, we evaluate the chiral condensate from the QCD vacuum with additional monopoles.

The numerical results clearly show that the values of the chiral condensate gradually decrease by increasing the values of the monopole charges as shown in Fig. 6. This is an evidence that monopoles are closely related to the chiral symmetry breaking.

7 Quark masses and monopoles

Lastly, we evaluate the quark masses $\bar{m} = \frac{m_u+m_d}{2}$ and m_s based on Refs. [30, 31].

In this study, we use the experimental results of the decay constant and the mass of K meson as the input values; $f_{K^-}^{Exp.} = (156.2 \pm 0.2 \pm 0.6 \pm 0.3)$ [MeV] (2013) and $m_{K^-}^{Exp.} = 493.677 \pm 0.013$ [MeV] (2014) (Particle Data Group). We determine the scale of our system. The scale is $a^{-1} = 2.00(8)$ [GeV]. We do not consider the errors of the experimental results in our calculations.

We then evaluate the quark masses considering the renormalization constant. The results of the quark masses in $\overline{\mathrm{MS}}$-scheme at 2 [GeV] using normal QCD vacuums are

$$\bar{m}^{\overline{MS}}\ (2\ \mathrm{GeV}) = 4.0(4)\ \ [\mathrm{MeV}], \tag{8}$$
$$m_s^{\overline{MS}}\ (2\ \mathrm{GeV}) = 98(9)\ \ [\mathrm{MeV}], \tag{9}$$
$$(a^{-1} = 2.00(8)\ \ [\mathrm{GeV}]).$$

The experimental results are

$$\bar{m} = 3.5^{+0.7}_{-0.2}\ \ [\mathrm{MeV}], \tag{10}$$
$$m_s = 95(5)\ \ [\mathrm{MeV}]\ \ (\mathrm{PDG}). \tag{11}$$

These results are consistent. The preliminary results in Fig. 7 show that the quark masses become gradually heavy by increasing the values of monopole charges.

8 Conclusions

We confirmed that the Overlap fermion preserves the chiral symmetry. We showed that the monopoles are related to instantons, the breakdown of the chiral symmetry, and the masses of the quarks, using the supercomputer SX-series. Especially, the monopoles may affect the masses of the quarks. This result indicates a possibility that the effects of monopoles can be detected in experiments. Now, we are checking the effects of the finite lattice volume and the discretization.

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We have carried out numerical simulations using the SX-ACE, SX-9, SX-8R, and PC clusters at the Cybermedia Center and the Research Center for Nuclear Physics at the University of Osaka. Moreover, we have used the SR16000 and the XC40 at the Yukawa Institute for Theoretical Physics at the University of Kyoto. We really appreciate their technical supports and the computational time.

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