Hadron Spectroscopy in Lattice QCD with Dynamical Quark Loops

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Hadron mass calculations are carried out in lattice QCD on a $9^3 \times 18$ lattice for flavor-nonsinglet mesons and baryons. Dynamical quark loops are fully incorporated with the Langevin technique. The contribution of dynamical quark loops significantly modifies the hadron masses in lattice units, but its dominant part can be absorbed into a shift of the coupling constant for the quark mass range we explored.

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Substantial progress has been made over the past couple of years in developing techniques for incorporating dynamical quark loops in the simulation of lattice QCD.[1-4] Especially promising seems to be the Langevin method[3,4] and its variants.[5] The main motive for developing those methods is to calculate hadron masses and other spectroscopic observables without recourse to the quenched approximation.[6] In this note we report our initial attempt in this direction using the Langevin simulation. Working on a $9^3 \times 18$ lattice with the Wilson quark action, we have found that, for the range of the hopping parameter we explored, most of the contribution from vacuum quark loops, while it substantially modifies the hadron mass values in lattice units, can be absorbed into a shift of the coupling constant. We also discuss briefly various technical questions that we encountered in applying the Langevin procedure for hadron spectroscopic calculations.

In applications of the Langevin procedure, the most problematical point is the presence of a systematic shift of the equilibrium distribution due to a finite Langevin time step $\Delta\tau$.[3,4,7] Particularly troublesome is the shift involving the lattice Dirac operator D. For long-wavelength modes, this is typically of the order of $(\Delta\tau)\lambda_{\min}^{-n}$ with $\lambda_{\min}$ the minimum eigenvalue of D and n a positive integer depending on the scheme. Since $\lambda_{\min}$ decreases toward light-quark masses, a large contribution from this term might seriously distort the distribution of long-wavelength modes. In the second-order scheme proposed in Ref. 3, the stochastic differential equation contains an $n=2$ piece, but an equilibrium distribution correct to order $[(\Delta\tau)D^{-2}]^2$ is ensured. On the other hand in the scheme of Ref. 4, while only terms with $n=1$ appear in the stochastic equation, the equilibrium distribution is correct only up to $O(\Delta\tau)$. A second-order Runge-Kutta algorithm similar to that of Ref. 3 can be devised which removes the integrable shifts of order $\Delta\tau$. There remains, however, the nonintegrable shift[8] which is of order $(\Delta\tau)\lambda^{-2}$. We have examined the magnitude of the error induced by the shifts by a change of $\Delta\tau$, and found that it is less severe with the scheme of Ref. 4 for light-quark masses. We have therefore employed this algorithm, with the integrable shifts of order $\Delta\tau$ removed by a Runge-Kutta algorithm, for the simulation reported here.

We have used the single-plaquette gauge action and the Wilson quark action. The gauge group is SU(3) and the number of flavors $N_f=2$ with the same hopping parameter K. We worked on a $9^3 \times 18$ lattice with periodic boundary conditions for the gauge and quark variables. Choice of the gauge coupling $\beta = 6/g^2$ requires some care; the quark loops generally render the gauge configuration more ordered, and hence the lattice size effectively shrinks toward light-quark masses. The value of β should be such that the finite-size effect for the gauge configuration is insignificant even then. We have decided on the value $\beta = 5.5$ which is above the near transition[9] of the pure gauge sector for heavy quarks. We did not observe any signature of finite-size effect in our simulation except possibly at the largest hopping parameter.

In order to generate equilibrated gauge configurations, 5000 iterations were carried out at $K=0.14$, 0.15, 0.155, 0.16, and 0.162. The Langevin time step was chosen to be $\Delta\tau = 0.01$ on the basis of an analysis of the minimum eigenvalue of the operator $\gamma_5 D$. (Another 6000 iterations with the pure gauge action were also made to compare the quenched calculation with the full QCD case.) The bulk of the computer time is spent in solving the linear equation $Dx=\eta$ with η the quark white noise. For this purpose we used the ILUCR scheme developed by Oyanagi.[10] This is a conjugate residual method combined with a preconditioning of D and a further acceleration similar to SOR. On a $9^3\times 18$ lattice a single conjugate residual iteration takes 1.2 sec on a HITAC S810/10. The iteration was continued until the residual $|r| = |\eta - Dx|$ becomes less than unity. This corresponds to 1% accuracy in each element of the vector x. Increasing the accuracy does not change the expectation value of observables beyond the statistical error. The number of iterations needed to meet $|r| < 1$ increased from about 6 at $K=0.14$ to about 50 at $K=0.162$.

The equilibration of the gauge configuration was monitored by measurement of both the hadron propagators and the Wilson loops. We found that the initial 1500 iterations were almost enough for equilibration and discarded the initial 2000 iterations. The average was taken at every 100 iterations for hadron propagators. Examination of the autocorrelation with respect to iterations of hadron propagators and Wilson loops has shown that all these correlations decrease to 0.1 or less after 300 to 500 iterations.

For the hadron operators we used the standard local relativistic forms, $\pi=\bar{u}\gamma_5 d$, $\boldsymbol{\rho}=\bar{u}\boldsymbol{\gamma} d$, $N=({}^t uC\gamma_5 d)u$, and $\boldsymbol{\Delta}=({}^t uC\boldsymbol{\gamma} u)u$. In the mass calculation with dynamical quark loops, one has to bear in mind that hadrons generally are no longer stable and the decays are allowed. The largest hopping parameter we could explore corresponds to $m_\pi a \sim 0.4$ and is above the thresholds for $\rho \to \pi\pi$ and $\Delta \to N\pi$. Therefore all hadrons are still stable and the standard procedure applies for extraction of hadron masses if the effect of the continuum is small. We have thus fitted the propagator data by a single exponential for baryons over the temporal separation $t=6$–9 and by a single hyperbolic cosine for mesons over $t=5$–13. The quality of the fit was generally excellent.

Our data for hadron masses is exhibited in Fig. 1 for π and in Fig. 2 for ρ, N, and Δ, together with their quenched values. We have estimated the error by dividing the propagator data into sets of ten and estimating the mass for each set. In Fig. 3 we present the temporal Wilson loop up to 4×4 as a function of K.

The data in Figs. 1–3 show that the effect of vacuum quark loops becomes quite sizable as K increases. For instance the hadron masses at $K\sim 0.16$ are reduced to about half of the quenched values. The critical hopping parameter K_c obtained by a linear extrapolation of m_π^2 in $1/K$ decreases to $K_c=0.1635\pm 0.0012$ from the quenched value $K_c=0.1844\pm 0.0009$. One may also extrapolate m_ρ linearly in $1/K$ to find the change in the lattice spacing a at the physical hopping parameter K_{phys} at which $m_\pi=135$ MeV and $m_\rho=770$ MeV. We find $a^{-1}=1.34$ GeV (0.15 fm) as compared to the quenched value $a^{-1}=0.99$ GeV (0.20 fm). Our fit of π and ρ masses versus hopping parameter for the full QCD case is summarized as

$$(m_\pi a)^2=(2.870\pm 0.145)(1/K-1/K_c),$$

$$m_\rho a=(1.351\pm 0.110)(1/K-1/K_c) + (0.575\pm 0.045).$$

A possible source of systematic error in our hadron

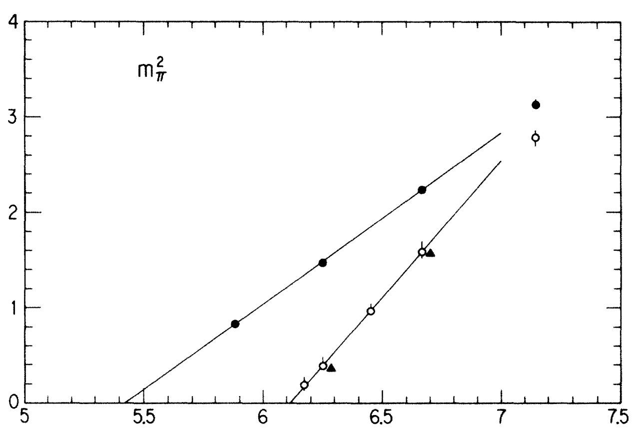

FIG. 1. Pion mass squared m_π^2 in lattice units as a function of $1/K$. The open and filled circles represent the full QCD and quenched results, respectively, at $\beta=5.5$. The triangles are the quenched results at a shifted β values (see text).

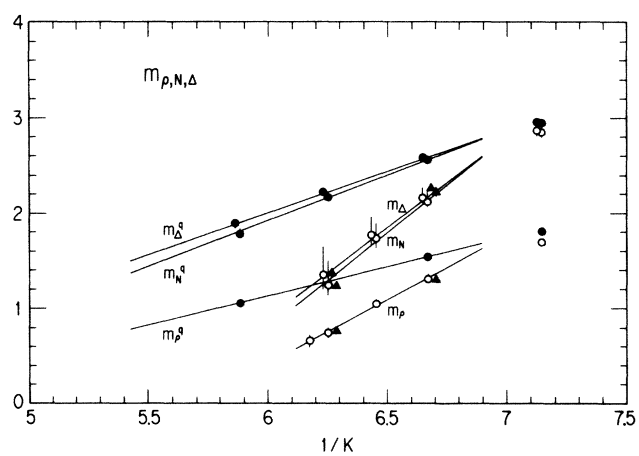

FIG. 2. Rho meson mass m_ρ, nucleon mass m_N, and delta mass m_Δ in lattice units as a function of $1/K$. The meaning of symbols is the same as in Fig. 1. Superscript q denotes the quenched mass value.

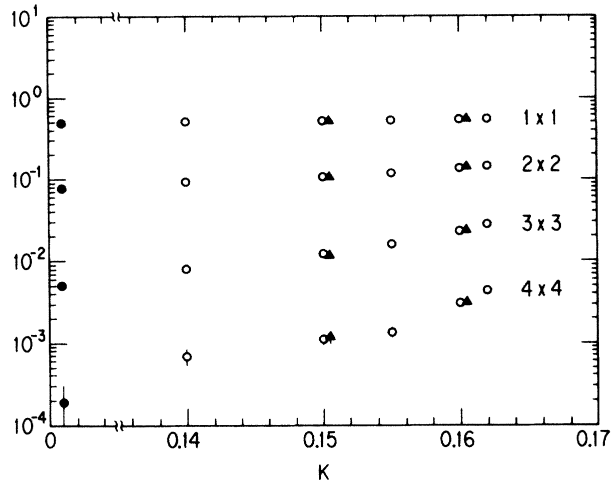

FIG. 3. Temporal Wilson loop as a function of K. The open circles are the full QCD results. The filled circles at $K=0$ and the triangles at $K=0.15$ and 0.16 represent the pure gauge average at $\beta=5.5$ and at shifted values $\beta=5.62$ and 5.75.

mass data is that the spatial size of the lattice $9\times a$ might not be large enough to contain a hadron inside the lattice. From a study using different boundary conditions, we found that such an error is smaller than statistical for mesons, but it may be appreciable for baryons. (This is not peculiar to full QCD and an error of similar magnitude is also seen in our quenched results.) If we extrapolate N and Δ masses linearly in $1/K$ we find

$$m_N a=(2.004\pm0.253)(1/K-1/K_c)+(1.026\pm0.122),$$

$$m_\Delta a=(1.895\pm0.328)(1/K-1/K_c)+(1.120\pm0.167),$$

and hence at $K=K_{\rm phys}$, $m_N/m_\rho=1.78\pm0.18$, and $m_\Delta/m_N=1.09\pm0.03$. These may be compared with the quenched values $m_N/m_\rho=1.76\pm0.10$ and $m_\Delta/m_N=1.09\pm0.04$.

An important quantitative question is how the effect of quark loops manifests itself and how it modifies the result of the quenched (valence) approximation. To answer this question, we first examine the magnitude of the effective shift $\Delta\beta$ of the coupling constant β due to vacuum quark loops. Table I exhibits $\Delta\beta$ estimated by matching of our Wilson-loop data for the sizes 1×1 to 4×4 to those of the pure-gauge data of Barkai, Moriarty, and Rebbi.[11] The good agreement of $\Delta\beta$ from various sizes of the Wilson loop suggests that the dominant part of the loop effect may be absorbed

TABLE I. The effective shift $\Delta\beta$ of the coupling constant estimated by matching the temporal Wilson loop of full QCD to that of the pure gauge sector.

	$K=0.14$	$K=0.15$	$K=0.16$	$K=0.162$
$W_{1\times1}$	0.06 ± 0.01	0.12 ± 0.01	0.24 ± 0.01	0.28 ± 0.01
$W_{2\times2}$	0.06 ± 0.01	0.12 ± 0.01	0.24 ± 0.01	0.28 ± 0.01
$W_{3\times3}$	0.06 ± 0.01	0.13 ± 0.01	0.25 ± 0.01	0.29 ± 0.01
$W_{4\times4}$	0.11 ± 0.03	0.15 ± 0.01	0.25 ± 0.01	0.30 ± 0.01

into a shift of the coupling β. (The value of the shift $\Delta\beta$ at $K=0.14$ is almost expected from an effective hopping-parameter expansion[12] to order K^{12}, but that at $K=0.16$ is a factor 2 larger than is expected from this expansion.) To verify this point we made hadron mass calculations in the quenched approximation at $K=0.16$, $\beta=5.75$ $(\Delta\beta=0.25)$ and at $K=0.15$, $\beta=5.62$ $(\Delta\beta=0.12)$, and have shown the results in Figs. 1–3. The agreement of the hadron masses between the full and quenched (with shifted β) calculations is excellent. Possible systematic deviation is not detected with our statistical accuracy. The chiral order parameter $\langle\bar\psi\psi\rangle$ was also found to agree between the two calculations. Therefore we conclude that the main effect of the vacuum quark loops is absorbed into a shift of the coupling for the quark mass range heavier than the decay thresholds for $\rho\to\pi\pi$ and $\Delta\to N\pi$. This feature of the full QCD calculation underlies the qualitative success of the quenched approximation[13] for the mass spectrum of flavor-nonsinglet mesons and baryons.

At a more quantitative level, however, the fact that the quenched calculation accurately reproduces the result of full QCD means that the inclusion of the vacuum-quark-loop effects cannot solve the problems known in the quenched calculation; the problem of a large m_N/m_ρ ratio and a small $\Delta-N$ mass difference still remains in our full QCD result. Hence these problems are not ascribable to the quenched approximation but are more likely to come from the common sources which affect the simulations done so far; insufficient size of the lattice as compared to the size of hadrons is one problem we have already mentioned. The minimum momentum might be large compared to the typical momentum with hadrons. The difficulty of carrying out the simulation for really small quark mass necessitates an extrapolation which not only introduces ambiguities but also might miss important information such as opening of decay thresholds which occurs at $m_\pi a\sim0.2$ in our case. To give the simulation a realistic predictive power, one has to work on a larger lattice at a weaker coupling and make a simulation at much smaller quark mass values. These requirements necessitate a further improvement of the computing algorithms and a sizable increase of the computing power over what is available at present.

The numerical calculation was carried out on a HITAC S-810/10 at the National Laboratory for High Energy Physics (KEK). We are greatly indebted to S. Kabe, T. Kaneko, and R. Ogasawara for assistance in operating the computer, and to the Theory Division of KEK for warm hospitality. We are particularly grateful to H. Sugawara and T. Yukawa for their strong support for our work. We would also like to thank Y. Iwasaki for informative discussions on the quenched hadron-mass calculation.

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