Hadronic molecules in lattice QCD

Chris Stewart and Roman Koniuk
Department of Physics and Astronomy, York University, 4700 Keele Street, Toronto, Ontario, Canada M3J 1P3
(Received 17 November 1997; published 7 April 1998)

An adiabatic approximation is used to derive the binding potential between two heavy-light mesons in quenched SU(2)-color lattice QCD. Analysis of the meson-meson system shows that the potential is attractive at short and medium range. The numerical data is consistent with the Yukawa model of pion exchange. [S0556-2821(98)02911-7]

PACS number(s): 12.38.Gc, 12.38.Aw, 24.85.+p

I. INTRODUCTION

Quantum chromodynamics is widely accepted as the correct theory of quark-quark interactions. QCD effective theories such as chiral perturbation theory have successfully described a wide range of hadronic phenomena. Nucleon-nucleon interactions, for example, have traditionally been modeled by effective meson-exchange theories. Such theories are long-range approximations to QCD interactions mediated by gluons and quark pairs. A derivation of the strong nuclear force from full QCD is obviously desirable.

Lattice QCD provides a first-principles framework for such a derivation. However, the nucleon-nucleon system, containing six light quarks, is well beyond the current limits of computation. In fact, at first sight such a computation seems impossible—lattice QCD is providing physical hadronic data consistent with experiment at the ~5% level. The nuclear physics problem, the interaction between two color-neutral objects, is an effect two or three orders of magnitude smaller. Nevertheless, nuclear models involving static quark clusters in unquenched QCD [1] and light-quark hadrons in confining QED_{2+1} [2] have been examined, and both give encouraging results. An unquenched lattice QCD simulation of the nucleon-nucleon system is doubtless some years away. In this paper we examine the same fundamental problem in a simpler setting, by examining the interactions between two heavy-light mesons [3].

An elementary problem in molecular physics is the derivation of the binding energy of the H_2 molecule. A good first approximation can be found by using an adiabatic approximation, in which the (slow) nuclear kinematics are removed by treating each nucleus as a static force center, and the remaining (fast) electronic problem is solved as a function of the nuclear separation. This generates an effective potential for the two nuclei, which can be used as input for the inter-nucleon wave functions and energy levels.

We wish to consider an analogous problem—a ''hadronic molecule'' consisting of two heavy-light mesons, in which the heavy quarks are treated as static color sources, playing the role of the (slow) atomic nuclei. The gluons and light-quarks play the role of the fast degrees of freedom. In addition to the static heavy-quark gluon-exchange interaction, this calculation will include the effects of interactions between gluons and light-quarks, as well as light-quark exchange. The total energy of the system can be found from the asymptotic long-time behavior of the meson-pair propagator. An effective potential is extracted as a function of the meson separation.

The system described above contains only two light valence quarks. As such, we are still quite removed from a direct simulation of the nucleon problem. However, as all nuclei are hadronic molecules, our qualitative conclusions should be somewhat universal. Simulations of MM and $M\overline{M}$ systems are of further interest because of their immediate application to $K\overline{K}$ phenomena. Studies of multi-quark states indicate that the only likely bound four-quark systems are mesonic molecular states [4]. Two exotic particles, the $a_0(980)$ and $f_0(975)$, are thought to be lightly bound $K\overline{K}$ molecules [5].

This paper describes a lattice simulation of heavy-light mesonic molecules, using SU(2)-color quenched QCD for computational simplicity. We consider both meson-meson and meson-antimeson systems. The next section describes the meson operators used in this simulation, and outlines the various contributions to the meson-pair propagators. In Sec. III we list the lattice actions used and the values of simulation parameters, and our results are given in Sec. IV.

II. OPERATORS AND PROPAGATORS

We used a local pseudoscalar meson operator,

$$M(\vec{x},t)=\overline{\psi_l}(\vec{x},t)\gamma_5\psi_h(\vec{x},t)\,, \tag{1}$$

constructed from heavy (h) and light (l) Wilson quarks. With quark propagators given by

$$G(\vec{x},t;0,0)=\langle 0|\psi(\vec{x},t)\overline{\psi}(0,0)|0\rangle\,, \tag{2}$$

the zero-momentum meson propagator is then

$$\begin{aligned}G_M(t)&=\mathrm{Tr}\sum_{\vec{x}}G_h(\vec{x},t;0,0)\gamma_5 G_l(0,0;\vec{x},t)\gamma_5\\ &=\mathrm{Tr}\sum_{\vec{x}}G_h(\vec{x},t;0,0)G_l^\dagger(\vec{x},t;0,0)\,.\end{aligned} \tag{3}$$

The hopping-parameter expansion of the quark propagator [6] gives, in the limit of infinite quark mass,

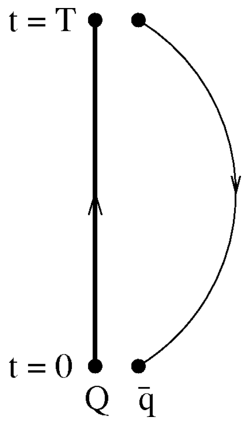

FIG. 1. Heavy-light meson propagator constructed from heavy (Q) and light (q) quark propagators.

$$G_h(\vec{x},t;0,0) \propto \delta^3_{\vec{x},0} \prod_{\tau=0}^{t-1} U_4(0,\tau) . \tag{4}$$

That is, the heavy-quark propagator becomes simply a string of gauge-field links in the time direction, and is calculated in one sweep of the lattice. Figure 1 shows a contribution to the heavy-light meson propagator.

An operator for a heavy-light meson-pair with spatial separation $\vec{R}$ is

$$\mathcal{O}_{MM}(\vec{R},t) = M(\vec{x},t)\ M(\vec{x}+\vec{R},t) . \tag{5}$$

The propagator for this system is then

$$G_{MM}(t,\vec{R}) = G_D - G_E , \tag{6}$$

where a sum over all contractions of the quark fields was performed, giving

$$\begin{aligned} G_D(t,\vec{R}) = &\ \mathrm{Tr}[G_h(0,t;0,0)G_l^\dagger(0,t;0,0)] \\ &\times \mathrm{Tr}[G_h(\vec{R},t;\vec{R},0)G_l^\dagger(\vec{R},t;\vec{R},0)] , \\ G_E(t,\vec{R}) = &\ \mathrm{Tr}[G_h(0,t;0,0)G_l^\dagger(\vec{R},t;0,0) \\ &\times G_h(\vec{R},t;\vec{R},0)G_l^\dagger(0,t;\vec{R},0)] . \end{aligned} \tag{7}$$

Note that, with the heavy-quark approximation (4), the separation $\vec{R}$ is well-defined throughout the propagation. Contributions to G_D and G_E, the direct and exchange terms, are depicted in Fig. 2.

The meson-antimeson propagator has a similar form,

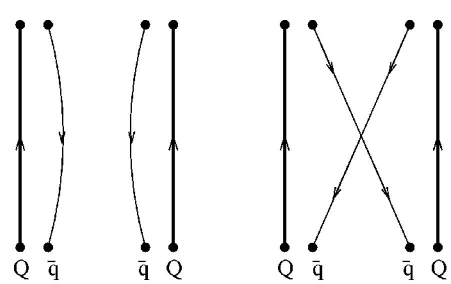

FIG. 2. (a) Direct and (b) exchange terms for MM system.

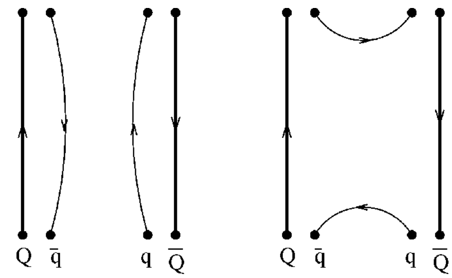

FIG. 3. (a) Direct and (b) exchange terms for $M\overline{M}$ system.

$$G_{M\overline{M}}(t,\vec{R}) = \mathcal{G}_D - \mathcal{G}_E , \tag{8}$$

where

$$\begin{aligned} \mathcal{G}_D(t,\vec{R}) = &\ \mathrm{Tr}[G_h(0,t;0,0)G_l^\dagger(0,t;0,0)] \\ &\times \mathrm{Tr}[G_l(\vec{R},t;\vec{R},0)G_h^\dagger(\vec{R},t;\vec{R},0)] , \\ \mathcal{G}_E(t,\vec{R}) = &\ \mathrm{Tr}[G_h(0,t;0,0)G_l^\dagger(\vec{R},t;0,0) \\ &\times G_h^\dagger(\vec{R},t;\vec{R},0)G_l(0,t;\vec{R},0)] . \end{aligned} \tag{9}$$

Contributions to these terms are shown in Fig. 3.

The ground-state energy of the two-meson system is extracted from the long-time evolution of the system's propagator [6]. Expanding the propagator as a sum over eigenstates of the Hamiltonian $|N\rangle$ with eigenvalues E_N, the propagator becomes proportional to the exponential of the ground-state energy E_0 for long times,

$$\begin{aligned} G(R,t) &= \langle 0|\overline{\mathcal{O}}_{MM}(\vec{R},t)\mathcal{O}_{MM}(\vec{R},0)|0\rangle \\ &= \sum_N \langle 0|\overline{\mathcal{O}}_{MM}(\vec{R},t)|N\rangle\langle N|\mathcal{O}_{MM}(\vec{R},0)|0\rangle \\ &= \sum_N |\langle 0|\overline{\mathcal{O}}_{MM}(\vec{R},0)|N\rangle|^2 e^{-E_N(R)t} \\ &\simeq c_0\ e^{-E_0(R)t} \quad \text{as} \quad t\to\infty . \end{aligned} \tag{10}$$

The binding energy $V(R)$ is then defined as the difference between the ground-state energy and the masses of the two independent mesons,

$$E_0(R) = 2m_M + V(R) . \tag{11}$$

III. SIMULATIONS

A model of quenched QCD with SU(2)-color was used to simplify analysis. The standard Wilson action for the pure gauge field is [6],

$$S_G = -\beta \sum_P \left(1 - \frac{1}{2}\mathrm{Tr}\ U_P\right) . \tag{12}$$

Here β is the inverse of the square of the coupling strength, and the sum is over all plaquettes on the lattice. The Wilson action for light quarks has the form

$$S_q = \sum_{n,m} \overline{\psi_n}\, K_{nm}\, \psi_m, \tag{13}$$

with the action matrix given by

$$K_{nm} = \delta_{n,m} - \kappa \sum_{\mu} [(1-\gamma_\mu) U_\mu(n) \delta_{n+\hat{\mu},m} + (1+\gamma_\mu)\, U_\mu^\dagger(n-\hat{\mu}) \delta_{n-\hat{\mu},m}]. \tag{14}$$

The light-quark propagator is then the inverse of the action matrix,

$$G_l(n,m) = K_{nm}^{-1}. \tag{15}$$

Simulations were performed on an 8^4 lattice with periodic boundary conditions. An ensemble of 400 gauge field configurations was generated with a Metropolis algorithm at $\beta=2.3$. Using the standard prescription for translating physical SU(3) QCD to unphysical SU(2) QCD, we used the pion and rho meson masses to set the lattice scale [7]. We found the lattice spacing to be roughly 0.2 fm, and the lattice is then ~1.6 fm along a side. One expects the radius of the heavy-light meson to be around half that of the pion, or ~0.5 fm, and so our lattice volume should be large enough to contain the two mesons.

To ensure statistical independence, 200 update sweeps were performed between stored configurations. Quark propagator matrix inversions (15) were performed with a conjugate gradient algorithm, at a value of $\kappa=0.165$ for the hopping parameter.

IV. RESULTS

All propagators under consideration are symmetric in time, since the periodic boundary conditions allow contributions from quarks and antiquarks winding around the lattice. The mass of the heavy-light meson was taken from fits to the meson propagator (3),

$$G_M(t) = c_M \cosh[m_M(t-T/2)], \tag{16}$$

where $T=8$ is the period of the lattice in the time direction. While this is an asymptotic relation, valid for long times, in practice fits with acceptable χ^2 were obtained for $2 \leqslant t \leqslant 6$. The average mass obtained from these fits was

$$m_M = 0.969 \pm 0.008 \tag{17}$$

in lattice units.

A. The *MM* system

The meson-pair propagator, Eq. (6), was constructed for values of the separation R from 0 to 7 lattice spacings. Given that statistical fluctuations in the individual meson propagators will likely be highly correlated to fluctuations in the MM-system propagator, we were able to reduce statistical errors by analyzing the ratio

$$C(\vec{R},t) = \frac{G_{MM}(\vec{R},t)}{G_{M_1} G_{M_2}}. \tag{18}$$

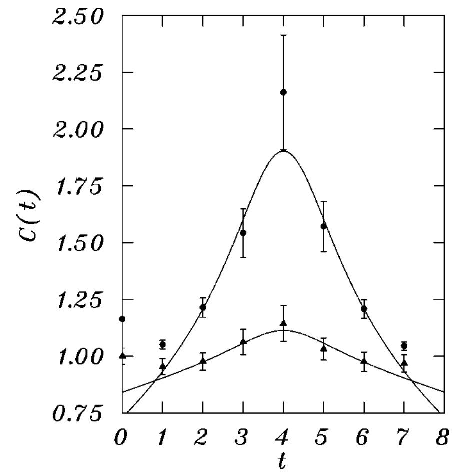

FIG. 4. Fits to the propagator ratio (19), for meson separation $R=0$ (circles) and $R=1$ (triangles). Error bars indicate jacknife errors.

For each value of the separation R, the configuration average of $C(\vec{R},t)$ was fit with a ratio of cosh functions,

$$C(R,t) = c_R \frac{\cosh^2([2m_M - V(R)]\tau)}{\cosh^2(m_M\, \tau)}, \tag{19}$$

with

$$\tau = t - \frac{T}{2}, \tag{20}$$

and using the meson mass given in Eq. (17). The results of the fit for $R=0$ and $R=1$ are shown in Fig. 4.

The binding potential extracted from Eq. (18) is shown in Fig. 5. The data has been fit with a periodic Yukawa function,

$$V(R) = a \left(\frac{e^{-\mu r}(1-e^{-r/d})}{r} + \frac{e^{-\mu(N-r)}(1-e^{-(N-r)/d})}{N-r} \right), \tag{21}$$

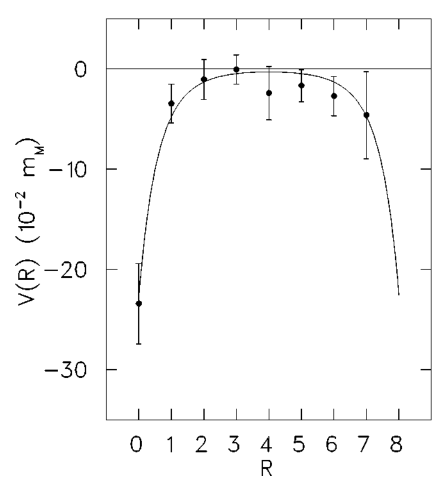

FIG. 5. MM potential $V(R)$ fit with a discrete Yukawa function (21).

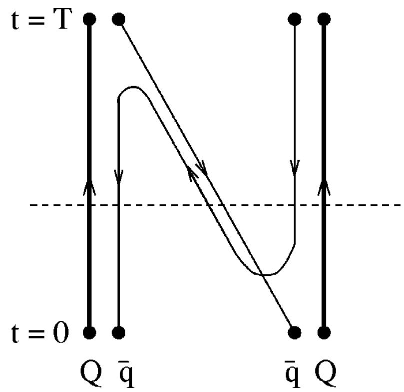

FIG. 6. A pion-exchange contribution to the MM propagator—at the time-slice indicated by the dotted line, two heavy-light mesons and a pion are present.

where N is the spatial length of the lattice. The parameter $d=d(N)$ provides the correct limiting behavior for $r=0$. This form reduces to the continuum Yukawa function as $N\to\infty$ $(d\to 0)$, and is in excellent agreement with numerical calculations of the discrete Fourier transform of $1/(k^2+\mu^2)$. We found $d\simeq 0.5$ at $N=8$, and using this in Eq. (21) we obtain [goodness-of-fit χ^2/(degree of freedom)$=0.5$]

$$a=(-12\pm 3)\times 10^{-2}\ m_M,$$

$$\mu=0.7\pm 0.4 \ \text{(lattice units)}. \tag{22}$$

The strength of this potential, described by the constant a, is consistent with nuclear potentials which are two orders of magnitude smaller than nucleon rest masses.

The potential is certainly attractive for small separations. Evidence for attraction at small separations was also seen in the staggered-quark calculation of Mihály *et al.* [3]. To ascertain whether the potential is significantly non-zero for meson spacings $R>0$, the data for $R=2$ to $R=6$ was fit with a constant function,

$$V(R)=c, \tag{23}$$

giving

$$c=(-1.3\pm 0.8)\times 10^{-2}\ m_M. \tag{24}$$

This constant term is more than one and a half standard deviations below zero, suggesting that there is some attractive potential even at medium-range separations. We regard the near-vanishing potential at the largest separations $(R=4)$ to be circumstantial evidence that our lattice volume is large enough to contain the meson-meson system.

The Yukawa parameters (22) correspond to a model of hadron interactions mediated by pion exchange, with the exchanged pion mass given by $m_\pi=\mu=0.7\pm 0.4$ in lattice units. Even though we are working in the quenched approximation and virtual $q\bar{q}$ pairs are absent, the exchange term in Eq. (6) will include pion exchange contributions—one such exchange is shown in Fig. 6.

Pion propagators were constructed using the same gauge field configurations at the same value of κ, to provide a pion mass for direct comparison with Eq. (22). The pion propagator is equivalent to Eq. (3), with two light-quark fields,

$$G_\pi(t)=\mathrm{Tr}\sum_n G_l^2(n,t;0,0), \tag{25}$$

and the pion mass was extracted from cosh fits to this propagator. The result of $m_\pi=0.38\pm 0.18$ agrees within errors with the Yukawa pion mass above.

B. The $M\bar{M}$ system

Simulations of a meson-antimeson system using Eq. (8) were performed. The results were not consistent with those described above for the MM system. The propagators tended to behave exactly like Wilson loops, just indicating that the system's ground state was a state where the light quarks have annihilated, leaving a static $Q\bar{Q}$ pair. Figure 3(b) shows a contribution from such a state. A proper simulation of $M\bar{M}$ systems may require a more realistic, dynamic treatment of the heavy quarks.

V. CONCLUSIONS

The binding potential between two heavy-light mesons in SU(2) QCD was found by considering the long-time behavior of propagators for the two-meson system. The heavy-quark approximation simplified analysis considerably, as the heavy quark plays a role analogous to the heavy nucleus in the adiabatic calculation of the binding potential in the H_2 molecule.

The binding potential derived in this study is attractive and short ranged, and periodic due to the boundary conditions of the lattice. The meson-meson interaction can be modeled by a pion-exchange Yukawa theory. Comparing our results with a Yukawa model, the potential has the correct form, and the exchanged pion mass derived from the potential agrees within errors with the pion mass calculated at the same values for the simulation parameters. While the large errors prompt caution, these results make us confident that the heavy-light meson-pair system is tractable in lattice QCD, and is a promising step towards a first principles treatment of the nuclear physics problem.

Unfortunately, in the $M\bar{M}$ propagator we only saw evidence of a static $Q\bar{Q}$ pair, due to the annihilation of the light quarks. Overlap with physical $M\bar{M}$ states would be enhanced if the heavy quarks were allowed to propagate spatially, perhaps in the regime of non-relativistic QCD. More work needs to be done to fully appreciate the subtleties of this system.

The very low light-quark mass used in this study ($\kappa=0.165$ gives a rho-pion mass ratio of $m_\rho/m_\pi\simeq 3.0$) resulted in large statistical fluctuations in the quark propagators, evidenced by the error bars in Fig. 5. Unfortunately, raising the quark mass leads to smaller contributions from light-quark exchange, and so weakens the resulting potential. These problems are in part due to the low-order approximations in the Wilson quark and gluon actions. We have commenced simulations using improved actions for the gauge fields [8,9] and fermion fields [10]. These actions remove most of the discretization errors, and restore much of the rotational symmetry of the continuum QCD action lost in the hypercubic lattice approximation.

[1] K. Rabitsch, H. Markum, and W. Sakuler, Phys. Lett. B **318**, 507 (1993).
[2] J.D. Canosa, H.R. Fiebig, and H. Markum, Nucl. Phys. B (Proc. Suppl.) **42**, 657 (1995).
[3] A. Mihály, H.R. Fiebig, H. Markum, and K. Rabitsch, Phys. Rev. D **55**, 3077 (1997).
[4] J. Weinstein and N. Isgur, Phys. Rev. Lett. **48**, 659 (1982).
[5] J. Weinstein and N. Isgur, Phys. Rev. D **41**, 2236 (1990).
[6] H.J. Rothe, *Lattice Gauge Theories—An Introduction* (World Scientific, Singapore, 1992).
[7] R. Woloshyn, Phys. Rev. D **34**, 605 (1986).
[8] K. Symanzik, Nucl. Phys. **B226**, 187 (1983).
[9] M. Alford, W. Dimm, G.P. Lepage, G. Hockney, and P. Mackenzie, Phys. Lett. B **361**, 87 (1995).
[10] M. Alford, T. Klassen, and P. Lepage, Nucl. Phys. B (Proc. Suppl.) **47**, 370 (1996).