Interactions between heavy-light mesons in lattice QCD

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A potential between heavy-light mesons is extracted from quark correlation functions in the framework of quenched lattice QCD with Kogut-Susskind fermions. We show that the resulting potential is attractive at short distances. An analysis of the influence of the light quark mass on the interaction is performed. [S0556-2821(97)06005-0]

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I. INTRODUCTION

The nucleon-nucleon interaction has been parametrized by boson-exchange models for several decades. On the other hand, quantum chromodynamics (QCD) provides new degrees of freedom at the subnuclear level which should give insight into the nature of the nucleon-nucleon interaction and its underlying physics from first principles. The vacuum of QCD contains both virtual gluons and quarks. As a consequence the nucleon-nucleon forces are mediated for short distances by gluon exchange between the constituent quarks whereas for longer distances the production of quarkantiquark pairs is likely the dominating mechanism. The quark-antiquark exchange can be treated as an effective meson exchange leading to the construction of the Bonn and Paris potentials [1]. The meson-theoretical potentials give a satisfactory description of the nucleon-nucleon scattering data which are mainly sensitive to long range distances. The gluon exchange can be studied by phenomenological potential and bag models, allowing for an effective description of the interaction of the six-quark system [2].

Today the aim is to calculate the nucleon-nucleon forces directly from the field equations of QCD. Earlier calculations with static quarks have demonstrated that the potential between 2 three-quark clusters is attractive [3]. A hard repulsive core of the potential, as suggested by experiments and their interpretation, could not be observed in the region where the two nucleons have relative distance close to zero.

Recently a practical method to extract an effective hadron-hadron interaction has been applied within the framework of a (2+1)-dimensional QED (QED_{2+1}) lattice model [4,5]. Since this method employs dynamics, using quark propagators, antisymmetrization and quark exchange between the hadrons become possible. In this framework there is a repulsive core between the mesons, which are the only hadrons of QED_{2+1} . This encourages us to analyze the situation for QCD. In this paper we generalize the formalism to QCD_{3+1} and investigate the interaction between two heavy-light color singlets (*B* and *D* mesons). The role of the heavy quarks is to localize the mesons so that their relative distance \vec{r} becomes well defined. The computation of the potential is then based on two-meson time-correlation matrices.

II. LATTICE ACTION

The Euclidean lattice QCD action has the form

$$S(U, \overline{\chi}, \chi) = S_G(U) + S_F(U, \overline{\chi}, \chi), \qquad (2.1)$$

where

$$S_G(U) = \beta \sum_{\text{pl}} \frac{1}{3} \text{ReTr}(1 - U_{\text{pl}})$$
 (2.2)

is the SU(3) gauge action in Wilson's plaquette formulation and

$$S_F = \sum_{x,y} \overline{\chi}(x) G_{xy}^{-1}[U] \chi(y)$$
(2.3)

is the fermionic action in the Kogut-Susskind prescription [6]. Here $\overline{\chi}$ and χ are the staggered Grassmann fields. The fermionic matrix $G_{xy}^{-1}[U]$ is given by

$$G_{xy}^{-1}[U] = \frac{1}{2} \sum_{\mu} \left(\Gamma_{x\mu} U_{x\mu} \delta_{x+\mu,y} - \Gamma_{x-\mu\mu} U_{y\mu}^{\dagger} \delta_{x-\mu,y} \right)$$
$$+ m_f \delta_{x,y}, \qquad (2.4)$$

where m_f is the fermion mass and the phase factors $\Gamma_{x\mu}$ are reminiscent of the Dirac matrices.

III. MESON-MESON CORRELATOR

We define an appropriate set of operators for the twomeson system by generalizing the idea of Ref. [4] to (3+1)dimensional QCD with staggered fermions. Employing local interpolating operators for the heavy-light mesons, the onemeson fields with momentum $\vec{p} = (2\pi/L)(k_1, k_2, k_3)$ have the form

$$\phi_{\vec{p}}(t) = \frac{1}{V} \sum_{\vec{x}} e^{i\vec{p}\cdot\vec{x}} \overline{\chi}_{h}(\vec{x}t) \chi_{l}(\vec{x}t), \qquad (3.1)$$

where χ_l and χ_h are Grassmann fields with external flavors l (light quark) and h (heavy quark). This definition corresponds to a pseudoscalar particle in the Kogut-Susskind for-

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$$\Phi_{\vec{r}}(t) = \sum_{\vec{p}} e^{-i\vec{p}\cdot\vec{r}} \phi_{-\vec{p}}(t) \phi_{\vec{p}}(t).$$
(3.2)

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Correlations of these operators contain information about the dynamics of the meson-meson system and, ultimately, the effective residual interaction.

The two-point correlator, describing the propagation of *one* meson on the lattice, is

$$C^{(2)}(t,t_0) = [\langle \phi_{\vec{p}}^{\dagger}(t) \phi_{\vec{p}}(t_0) \rangle - \langle \phi_{\vec{p}}^{\dagger}(t) \rangle \langle \phi_{\vec{p}}(t_0) \rangle]_{\vec{p}=0}.$$
(3.3)

The four-point time correlation matrix describes the propagation of *two* interacting mesons on the lattice:

$$C_{\vec{r}s}^{(4)}(t,t_0) = \langle \Phi_{\vec{r}}^{\dagger}(t)\Phi_{\vec{s}}(t_0) \rangle - \langle \Phi_{\vec{r}}^{\dagger}(t) \rangle \langle \Phi_{\vec{s}}(t_0) \rangle.$$
(3.4)

Here \vec{r} and \vec{s} are *relative* separations of the meson-meson system. The expressions in Eqs. (3.3) and (3.4) can be worked out in terms of contractions between the Grassmann fields. We obtain

$$C^{(2)}(t,t_0) = \frac{1}{V^2} \left\langle \sum_{\vec{x}} \operatorname{Tr}(G^{(h)\dagger}_{\vec{x}t,\vec{x}t_0}G^{-}_{\vec{x}t,\vec{x}t_0}) \right\rangle, \qquad (3.5)$$

$$C_{\vec{r}}^{(4)}(t,t_{0}) = \frac{1}{V^{4}} \left\langle \sum_{\vec{x}} \left[\operatorname{Tr}(G_{\vec{x}t,\vec{x}t_{0}}^{(h)\dagger}G_{\vec{x}t,\vec{x}t_{0}}) \times \operatorname{Tr}(G_{\vec{x}+\vec{r}t,\vec{x}+\vec{r}t_{0}}^{(h)\dagger}G_{\vec{x}+\vec{r}t,\vec{x}+\vec{r}t_{0}}) - \operatorname{Tr}(G_{\vec{x}t,\vec{x}t_{0}}^{(h)\dagger}G_{\vec{x}+\vec{r}t,\vec{x}+\vec{r}t_{0}}) \times G_{\vec{x}+\vec{r}t,\vec{x}+\vec{r}t_{0}}^{(h)\dagger}G_{\vec{x}t,\vec{x}+\vec{r}t_{0}}) \right] \right\rangle$$
$$= C^{(4A)} - C^{(4B)}, \qquad (3.6)$$

where the trace is taken over the color indices of the propagator products. The superscript (h) denotes the heavy-quark propagators. Those can be obtained from a hoppingparameter expansion [7]. We only take the lowest order of the expansion so that the heavy quarks represent fixed color sources. Thus the heavy-quark propagator is given by

$$G_{\vec{x}t,\vec{x}t_0}^{(h)} = \left(\frac{1}{2m_h a}\right)^k [\Gamma_{\vec{x}4}]^k \prod_{j=1}^k U_{x=(\vec{x},ja),\mu=4}, \quad (3.7)$$

with a similar expression for the antiquark propagator. The heavy-quark mass m_h only gives rise to an irrelevant multiplicative factor in the static approximation and is set to $m_h a = 1$. The phase factors $\Gamma_{\vec{x}4} = (-1)^{(x_1+x_2+x_3)/a}$ in the Kogut-Susskind formulation are remnants of the Dirac matrices and $k = (t-t_0)/a$. As $G_{\vec{y}t,\vec{x}t_0}^{(h)} \equiv 0$ for $\vec{x} \neq \vec{y}$, all off-diagonal elements of the correlation matrix (3.4) vanish.

The diagrams contributing to Eq. (3.6) are shown in Figs. 1 and 2; the solid and wavy lines denote the heavy- and



FIG. 1. Diagram contributing to pure gluon-exchange part $C^{(4A)}$. Solid and wavy lines represent heavy and light quark propagators, respectively.

light-quark propagators, respectively. Figure 1 corresponds to the pure gluon-exchange part while Fig. 2 corresponds to the flavor-exchange part of the mesonic interactions.

The mass m of one heavy-light meson can be extracted from the behavior of the two-point correlator in large Euclidean time:

$$C^{(2)}(t,t_0) \propto e^{-m(t-t_0)}$$
. (3.8)

The ground-state energy of the meson-meson system can be extracted from the large Euclidean time behavior of the fourpoint correlator following quantum-mechanical reasoning [7,8]. Similar arguments for composite particles were presented in [5,9]. In the Euclidean formulation of quantum mechanics the spectral decomposition of the four-point Green function representing the two-meson system is

$$C_{\tau s}^{(4)}(t,t_0) = \sum_n \langle \Phi_{\tau}^{\dagger} | n \rangle \langle n | \Phi_{s} \rangle e^{-E_n(t-t_0)}.$$
(3.9)

 E_n are the energy eigenvalues and $|n\rangle$ the associated eigenstates. For a given potential we can solve the Schrödinger equation to obtain E_n and $|n\rangle$ and calculate the sum in Eq. (3.9). We invert this process and calculate the potential from a given Green function. As the heavy quarks lead to a localization of the mesons during the time evolution of the system, we have $|\vec{r}| = |\vec{s}| = r$, giving

$$C_r^{(4)}(t,t_0) = \sum_n |\langle \Phi_r^{\dagger} | n \rangle|^2 e^{-E_n(t-t_0)}.$$
 (3.10)

Since the correlation matrix $C^{(4)}$ describes the time evolution of the meson-meson system with a constant particle separation *r* for the whole process, we can extract the energy of two heavy-light mesons from the asymptotic time behavior at fixed *r* [5,7–9]:

$$C_r^{(4)}(t,t_0) \propto c_4(r) e^{-W(r)(t-t_0)}.$$
 (3.11)



FIG. 2. Diagram contributing to flavor-exchange part $C^{(4B)}$. Solid and wavy lines represent heavy and light quark propagators, respectively.



FIG. 3. Time dependence of the computed correlation functions and fits to $C^{(2)}$ and $C^{(4)}_{r=0}$ with $m_f a = 0.1$ (see text). For $C^{(2)}$ the errors are of the size of the symbols.

W(r) contains the interaction between the mesons and the kinetic energy of the light quarks as well as the intrinsic potential energy of the mesons. Since the heavy-light mesons considered here do not propagate in space, the relative kinetic energy of the mesons drops out of the theory in the sense that the Hamiltonian of the meson-meson interaction becomes identical with the interaction potential V(r) = W(r) - 2m. It is related to Eqs. (3.11) and (3.8), which can be extracted from QCD by computing the correlators (3.6) and (3.5).

IV. NUMERICAL RESULTS

The gauge field configurations of pure QCD were generated on a periodic $N_s^3 \times N_t = 8^3 \times 16$ lattice with inverse gauge coupling $\beta = 5.6$. According to the renormalization group equation this corresponds to a lattice spacing $a \approx 0.19$ fm. The results in this paper were obtained from an analysis of 100 configurations separated by 200 updates of the gauge fields. For the smallest quark mass 200 configurations were produced to improve statistics. The light-quark propagators with different mass parameters $m_f a$ in the range 0.025-0.2 were determined from the inversion of the fermionic matrix (2.4) using the conjugate gradient algorithm with 32 random sources [10]. To reduce the computational effort we do not average over different values of t_0 in the inversion process.

The light-quark propagators obtained by the inversion contain contributions both from (anti)quarks winding around the periodic lattice. To improve our statistics we took into account also heavy-quark propagators winding in the opposite direction for separations larger than $N_t/2$. In this way the correlators become symmetric about the center of the time axis.

We calculated the four-point propagator for different values of the meson separation r/a from 0 to 4 averaging over all spatial directions. Noninteger distances $r/a = \sqrt{2}, \sqrt{3}$, etc., were also included in order to estimate systematic errors on W(r) related to violation of rotational O(3) invariance by the lattice.

The potential was extracted from cosh fits to the correla-



FIG. 4. Meson-meson energies W(r) for several light-quark masses. Data points at degenerate distance r/a=3 are slightly shifted. The error bars were obtained by taking into account the statistical errors in the fit. Lines connecting the symbols are to guide the eye.

$$C^{(2)}(t) = \sum_{n} A_{n} \cosh[m_{n}(t-8a)] + (-1)^{t/a} \sum_{n} \widetilde{A}_{n} \cosh[\widetilde{m}_{n}(t-8a)], \quad (4.1)$$

$$C_{r}^{(4)}(t) = \sum_{n} B_{n}(r) \cosh[W_{n}(r)(t-8a)] + (-1)^{t/a} \sum_{n} \widetilde{B}_{n}(r) \cosh[\widetilde{W}_{n}(r)(t-8a)].$$
(4.2)

The terms alternating in sign are a peculiarity of the Kogut-Susskind formulation of lattice fermions and correspond to contributions from intermediate states of opposite parity. A precise analysis is needed in order to estimate the number of excited states contributing to the sums in Eqs. (4.1) and (4.2)(see, e.g., [11]). We analyzed the correlation functions by using fewer data points corresponding to asymptotic times and looked at the stability of the potentials from the fit. It turned out that the contribution from excited states does not alter the shape of the potential considerably, but fewer data points for the fit yield larger error bars in the potential. Thus, we included all points in a time direction to extract the lowest contribution from both terms in Eqs. (4.1) and (4.2), risking overestimating the mass parameters. However, it turned out that a four-parameter fit of $A_1, m_1, \overline{A_1}, \overline{m_1}$ and $B_1(r), W_1(r), \widetilde{B}_1(r), \widetilde{W}_1(r)$ gives a satisfactory result with an acceptable χ^2 . As an example, in Fig. 3 we show the numerical results for the two-point correlator as well as for the four-point correlator at r=0 with $m_f a=0.1$, and fits to the data points. The Levenberg-Marquardt method described in [12] was employed. The solid curves correspond to the functions in Eq. (4.1) with the parameter set $A_1, m_1, \widetilde{A_1}, \widetilde{m_1}$ and in Eq. (4.2) with $B_1(0), W_1(0), \tilde{B}_1(0), \tilde{W}_1(0)$, respectively. Note that one correlation function is represented by two curves distinguishing between even and odd distances. The mass of the meson is identified by $m = m_1$ and the meson-meson energy by $W(r) = W_1(r)$.

A comparison of the direct term $C^{(4A)}$ and the quarkexchange term $C^{(4B)}$ indicates a leading contribution from $C^{(4A)}$ being almost an order of magnitude larger than $C^{(4B)}$. The reason is that due to the strong confining force the possibility for light valence quarks to be exchanged between the mesons is very small.

In Fig. 4 we show the results of W(r) for different lightquark mass parameters. The horizontal lines correspond to the energies 2m of two independent mesons. The error bars were obtained by taking into account the statistical errors of the correlators $C^{(2)}$ and $C^{(4)}$ in the fit and estimating the covariance matrix of the standard errors in the fitted parameters (see [12]). For smaller m_f the error bars increase due to the inaccuracy of the inversion of the fermionic matrix. The curves reach their plateau at $r/a \approx 2$, continuing, with large fluctuations, to the asymptotic values 2m. To be numerically consistent with W(r) at large distances, the mass 2m of two



FIG. 5. Meson-meson potentials V(r) = W(r) - 2m for different light-quark masses m_f . Error bars are omitted and data at r/a=3 are averaged.

noninteracting mesons was extracted from fits to the square of the meson two-point function $[C^{(2)}]^2$. We should point out that interaction energies in Fig. 4 are only about 5×10^{-2} of a typical hadron mass. This is characteristic of residual hadronic forces.

The resulting potentials are collected in Fig. 5. The error bars are omitted and the data at distance r/a=3 are averaged for the sake of clarity of the figure. Attraction for short distances is evident. This is different for QED where the gauge group U(1) has only one internal degree of freedom leading to Pauli repulsion [4]. We find that the interaction is stronger for smaller light-quark masses, but its range is always approximately the same. Confinement forces suppress the exchange of quarks at large separations. Quark exchange plays a significant role only for distances r much less than 2a. The systematic deviations in the off-axis directions may originate from anisotropy effects of the cubic lattice.

V. CONCLUSIONS

A practical method to extract an effective hadron-hadron potential within the framework of lattice QCD has been developed and applied. The heavy-light approximation was chosen to make calculations easier, rather than to describe the interaction between real particles with certain quantum numbers. This simplification allowed us to take the effect of dynamical valence quarks into account and realize a correct antisymmetrization of the correlation functions. We were able to extract the potential from the Euclidean time behavior of these correlators in a direct way. Calculations from inverse scattering theory propose a similar shape for $K\overline{K}$ potentials [13]. This corresponds to an MM system consisting of a heavy-light meson and its antiparticle while in our study MM potentials have been considered. The choice of color group SU(3) brings us closer to our aim of extracting a potential between two nucleons from lattice QCD. Such a project necessitates the computation of a four-point hadron Green function which is equivalent to a correlation function of six-quark propagators within the QCD path integral.

An obvious next step in this program is to study the residual interaction of two light mesons. An independent lattice investigation using Wilson fermions is desirable because the assignment of quantum numbers to the interpolating operators is straightforward, and consequently physical particles are easily identified. A new simulation with an improved action [14] aiming at an extraction of the residual interaction closer to phenomenology is in progress [15].

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