Exploratory Study of Nucleon-Nucleon Scattering Lengths in Lattice QCD

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An exploratory study is made of the nucleon-nucleon s-wave scattering lengths in quenched lattice QCD with the Wilson quark action. The π-N and π-π scattering lengths are also calculated for comparison. The calculations are made with heavy quarks corresponding to $m_\pi m_\rho \approx 0.73$–$0.95$. The results show that the N-N system has an attractive force in both spin singlet and triplet channels, with their scattering lengths significantly larger than those for the π-N and π-π cases, a trend which is qualitatively consistent with the experiment. Problems toward a more realistic calculation for light quarks are discussed.

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The understanding of low energy nucleon-nucleon (N-N) interactions has been one of the most fundamental problems in nuclear physics. A large effort to construct elaborate meson exchange models has enabled us to describe the low energy N-N phase shifts and deuteron properties quite well [1]. However, these models are essentially phenomenological in that they use mesons and baryons as the basic degrees of freedom and choose the coupling strengths among them to fit the experimental data. Deriving the low energy properties of the N-N interaction directly from the dynamics of quarks and gluons is clearly a problem posed to numerical studies of lattice QCD.

An important parameter characterizing the low energy N-N interaction is the s-wave scattering length. The experimental values are listed in Table I [2] together with those for π-N and π-π cases for comparison. We observe that the N-N scattering lengths are markedly larger. We also note that the negative sign for the spin triplet channel reflects the presence of the deuteron bound state as follows from Levinson's theorem. The small values for the π-N and π-π cases are understood as a consequence of chiral symmetry for u and d quarks; current algebra and PCAC (partial conservation of axial-vector current) have successfully predicted the sign and magnitude [3]. Since no such constraint exists for N-N scattering, its large scattering lengths are dynamical phenomena of QCD.

TABLE I. s-wave scattering lengths in units of fm [2].

N-N	$^3S_1$	$-5.432(5)$
	$^1S_0$	$+20.1(4)$
π-N	$I = \frac{1}{2}$	$+0.245(4)$
	$I = \frac{3}{2}$	$-0.143(6)$
π-π	$I = 0$	$+0.37(7)$
	$I = 2$	$-0.040(17)$

An elegant method for calculating scattering lengths in lattice QCD is provided by the formula [4] relating the s-wave scattering length a_0 between two hadrons h_1 and h_2 to the energy shift $\delta E = E_{h_1 h_2} - (m_{h_1} + m_{h_2})$ of the two-hadron state at zero relative momentum confined in a finite spatial box of a size L^3. It is given by

$$\delta E = -\frac{2\pi a_0}{\mu L^3}\left[1 + c_1\frac{a_0}{L} + c_2\left(\frac{a_0}{L}\right)^2\right] + O(L^{-6}), \quad (1)$$

with $\mu = m_{h_1}m_{h_2}/(m_{h_1} + m_{h_2})$ and $c_1 = -2.837\,297$ and $c_2 = 6.375\,183$. The energy shift and hadron masses m_{h_1} and m_{h_2} can be extracted from hadron four- and two-point functions calculated through numerical simulations. Previous studies have shown the practical feasibility of the application of the formula for the case of π-π scattering both for $I = 2$ [5] and also for the technically more difficult case of $I = 0$ [6]. With the development of the technique to calculate hadron four-point functions [6], we have attempted an exploratory study of the N-N s-wave scattering lengths, which we report in this Letter.

A realistic calculation of N-N scattering lengths faces three basic obstacles. The large values of scattering lengths of order 10 fm to be obtained mean that lattice sizes much larger than 2–3 fm, which are accessible in current numerical simulations, will be needed to suppress $O(L^{-6})$ corrections neglected in (1). Another difficulty in the spin triplet channel is that the lowest scattering state orthogonal to the bound deuteron state has to be constructed to apply (1). Finally, statistical fluctuations in N-N four-point functions grow rapidly toward large time separations and small quark masses as we shall discuss in detail below. In order to avoid these problems in our initial study, we have carried out simulations for heavy quarks with $m_\pi/m_\rho \approx 0.73$–$0.95$ in the quenched approximation. We employ the Wilson quark action and work at the inverse coupling constant $\beta = 6/g^2 = 5.7$ which corresponds to the lattice spacing $a \approx 0.14$ fm. A calculation of π-N and π-π scattering lengths at the same

β is also carried out to compare them with the results for the N-N case.

The parameters of runs are tabulated in Table II. Gauge configurations are generated for the single plaquette action separated by 1000 sweeps of the pseudo-heat-bath algorithm. Calculations for the π-π and π-N cases are made on a $12^3 \times 20$ lattice, while for the N-N case we employ a 20^4 lattice anticipating larger scattering lengths. We extract the energy shift $\delta E = E_{h_1 h_2} - (m_{h_1} + m_{h_2})$ from the ratio of the hadron Green's functions,

$$R(t) = \frac{\langle \mathcal{O}_{h_1}(t)\mathcal{O}_{h_2}(t+1)\mathcal{O}_{h_1}(0)\mathcal{O}_{h_2}(1)\rangle}{\langle \mathcal{O}_{h_1}(t)\mathcal{O}_{h_1}(0)\rangle\langle \mathcal{O}_{h_2}(t+1)\mathcal{O}_{h_2}(1)\rangle}$$

$$\xrightarrow{t\to\infty} \exp(-\delta E t), \qquad (2)$$

where the operators for h_2 are shifted by one lattice unit in the temporal direction to avoid mixing of color-Fierz transformed contributions [6].

Quark propagators for the N-N case are calculated with a wall source at $t = 0$ or 1, fixing gauge configurations to the Coulomb gauge in all space-time. The Dirichlet boundary condition is employed in the time direction to avoid contamination from negative parity states propagating backward in time. Projecting out spin singlet and triplet combinations of the two nucleon system is made by nonrelativistically combining the upper components of the nucleon operator $N = ({}^t q C^{-1}\gamma_5 q)q$ taking account of isospin factors.

Calculation of the π-N and π-π four-point functions requires quark propagators connecting two arbitrary space-time sites. We handle this problem by the method proposed in our previous work [6]: Quark propagators are calculated with a wall source for every time slice without gauge fixing. The nucleon source operator for the π-N case, however, is fixed to the Coulomb gauge to increase the signal to noise ratio.

In Fig. 1 we show $R(t)$ for the spin singlet and triplet channels in the N-N case at $K = 0.160$ corresponding to $m_\pi/m_\rho = 0.85$. A clear signal with a positive slope is observed for both channels, which means attraction ($\delta E_{NN} = E_{NN} - 2m_N < 0$) as expected. Similar results are obtained at two other values of the hopping parameter $K = 0.15$ ($m_\pi/m_\rho = 0.95$) and 0.164 ($m_\pi/m_\rho = 0.73$). We extract the energy shift δE_{NN} by fitting $R(t)$
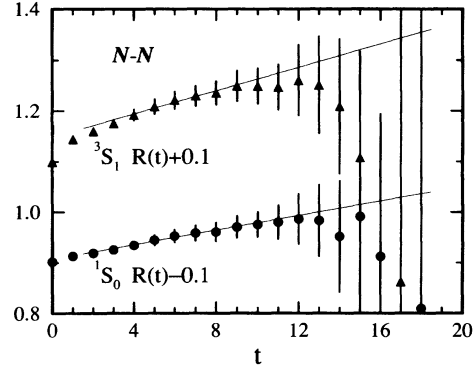

FIG. 1. $R(t)$ for the nucleon four-point function for the spin singlet and triplet channels at $\beta = 5.7$ and $K = 0.160$ on an $20^3 \times 20$ lattice in quenched QCD. Solid line is the linear fit to data over $4 \leq t \leq 9$.

with a linear form $R(t) = Z(1 - \delta E_{NN}t)$. The fitting range is chosen to be $4 \leq t \leq 9$ for $K = 0.150$ and 0.160. For the case of $K = 0.164$ we used $2 \leq t \leq 6$ for the fit due to the poor quality of our data. The fitted values of δE_{NN} are quite small (≈ 0.01), justifying the use of a linear function instead of an exponential.

For heavy quarks the N-N interaction becomes shorter ranged since pions exchanged between the nucleons are heavy, while the size of the nucleon will not be much reduced. In a simple potential model with a linear confining potential, for example, the hadron size scales as a third power of the constituent quark mass which is a slowly varying function of the hopping parameter. We may expect then that the deuteron becomes unbound for heavy quarks. Assuming this to be the case we can extract the scattering lengths through (1) for both spin singlet and triplet channels. The results, in lattice units, are tabulated in Table III. We should comment that the scattering lengths we found are large enough to warrant a repetition of the calculation with a larger lattice size even though we used quite a large size of 20^4. In fact, the three terms in formula (1) are comparable in magnitude for our results. We have not attempted such a finite-size analysis, as necessary simulations for larger lattice sizes exceed our computer resources.

Our results for the π-N and π-π four-point functions are plotted in Fig. 2 for $K = 0.164$. The data are also fitted with the linear form $R(t) = Z(1 - \delta E t)$ over $4 \leq t \leq 9$. The resulting scattering lengths are listed in Table III. (We could not extract the $I = 1/2$ π-N scattering length at $K = 0.1665$ due to large errors in our data; this point will be discussed below.) The predictions of current algebra and PCAC are given by

$$a_0(\pi\pi) = +\frac{7}{16\pi}\frac{\mu_{\pi\pi}}{f_\pi^2} \ (I = 0), \quad -\frac{1}{8\pi}\frac{\mu_{\pi\pi}}{f_\pi^2} \ (I = 2),$$

$$(3)$$

TABLE II.   Parameters of simulations. All runs are made at $\beta = 5.7$ in quenched QCD.

	K	Lattice size	No. conf
N-N	0.150	$20^3 \times 20$	20
	0.160	$20^3 \times 20$	30
	0.164	$20^3 \times 20$	20
π-N	0.164	$12^3 \times 20$	60
	0.1665	$12^3 \times 20$	30
π-π	0.164	$12^3 \times 20$	70

TABLE III. Scattering lengths in lattice units at $\beta = 5.7$ in quenched QCD. Numbers in square brackets are current algebra predictions evaluated with the measured values of m_π, m_N, and f_π with the tadpole-improved Z factor.

K		0.150	0.160	0.164	0.1665
m_π		1.0758(51)	0.6919(63)	0.5081(35)	0.3588(82)
m_ρ		1.1302(66)	0.8171(86)	0.7008(67)	0.588(20)
m_N		1.788(11)	1.302(13)	1.093(20)	0.951(42)
N-N	$^3S_1$	+10.8(1.2)	+9.0(1.6)	+10.8(9)	
	$^1S_0$	+9.2(1.3)	+7.3(1.9)	+8.0(1.1)	
π-N	$I = \frac{1}{2}$			+3.04(66)	$\cdots$
				[+2.59]	[+2.86]
	$I = \frac{3}{2}$			$-1.10(20)$	$-1.31(22)$
				[-1.29]	[-1.43]
π-π	$I = 0$			+3.02(17)	
				[+3.32]	
	$I = 2$			$-0.924(40)$	
				[-0.947]	

$$a_0(\pi N) = +\frac{1}{4\pi}\frac{\mu_{\pi N}}{f_\pi^2} \ (I = \tfrac{1}{2}), \quad -\frac{1}{8\pi}\frac{\mu_{\pi N}}{f_\pi^2} \ (I = \tfrac{3}{2}),$$

(4)

where $\mu_{\pi\pi} = m_\pi/2$ and $\mu_{\pi N} = m_\pi m_N/(m_\pi + m_N)$ are the reduced masses. We list in Table III the numerical values of these predictions for the values of m_π, m_N, and f_π measured in our simulations with the tadpole-improved renormalization factor for f_π [7]. Our results for the scattering lengths are consistent with these values within one standard deviation. It is somewhat surprising that the agreement holds even at quite heavy quarks corresponding to $m_\pi/m_\rho \approx 0.73$. (For the π-π scattering lengths a similar agreement has previously been reported [5,6].)

In Fig. 3 we plot the scattering lengths as a function of m_π/m_ρ. It is apparent that the N-N scattering lengths are substantially larger than the π-N and π-π scattering lengths already for a heavy quark corresponding to $m_\pi/m_\rho \approx 0.73$. Also noteworthy is the trend, albeit with sizable errors, that the values for the spin triplet channel are larger than those for the singlet channel, indicating a stronger attraction in the triplet channel, which is consistent with the existence of the deuteron bound state. We find these results to be encouraging, although the scattering lengths we obtained are still very small compared to the experiment: our results correspond to $a_0(NN) \approx 1.0-1.5$ fm in physical units with $a \approx 0.14$ fm determined from the ρ meson mass extrapolated to the chiral limit. These small N-N scattering lengths are most likely to arise from a short interaction range for heavy pions ($m_\pi \approx 0.7-1.5$ GeV) for which our simulations are made; we expect that they would increase if simulations would be made with a small quark mass [8].

Let us now discuss the issues for extension of the present work toward a more realistic case of light quarks. On the theoretical side, if the deuteron is a bound

state only for light enough quarks as assumed here, the scattering length for the triplet channel extracted from the lowest two-nucleon energy should diverge at the value of K corresponding to the bound state formation, beyond which we need to construct the lowest scattering state
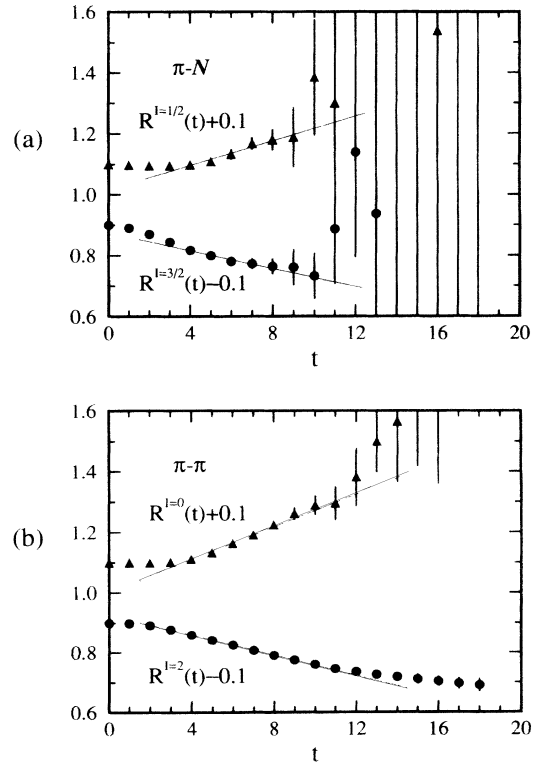

FIG. 2. $R(t)$ for the (a) π-N and (b) π-π four-point function at $\beta = 5.7$ and $K = 0.164$ on an $12^3 \times 20$ lattice in quenched QCD. Solid line is the linear fit to data over $4 \leq t \leq 9$.
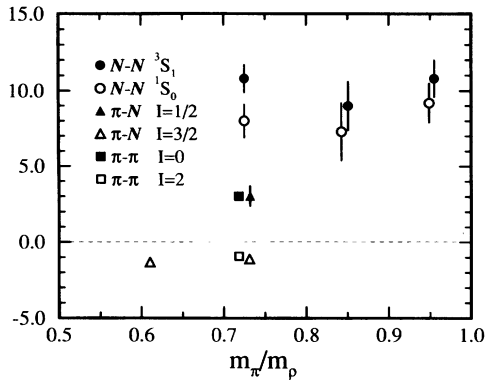
FIG. 3. Scattering lengths in lattice units at $\beta = 5.7$ in quenched QCD as a function of m_π/m_ρ.

orthogonal to the deuteron to extract the scattering lengths. Observing the diverging trend would be an interesting problem in its own light.

From the viewpoint of simulations, reducing statistical errors presents a major problem toward light quarks. A simple argument indicates that the error of $R(t)$ grows exponentially with t as $\delta R(t) \propto \exp[(2m_N - 3m_\pi)t]$ for the N-N four-point function; since the pion mass vanishes in the chiral limit while the nucleon mass stays nonzero, the slope $\alpha_{NN} = 2m_N - 3m_\pi$ becomes larger for lighter quarks. A rapid growth of error is clearly seen in Fig. 1; its t dependence is roughly consistent with the estimate. We also expect that the magnitude of errors increases for lighter quarks. Thus a progressively larger statistics is needed to obtain reliable results as the quark mass is decreased.

A similar situation holds for the π-N case. The estimated slope $\alpha_{\pi N} = m_N - m_\pi/2$ is even larger than α_{NN} for the range $K = 0.1665$–0.15, where we have made our simulation (e.g., $\alpha_{\pi N} = 0.84$ and $\alpha_{NN} = 0.66$ for $K = 0.164$). This explains a faster increase of errors with t for the π-N case [compare Fig. 1 and Fig. 2(a)]. An increase of magnitude of errors is also observed as the quark mass is reduced from $K = 0.164$ to $K = 0.1665$. This is the reason why we could not obtain the $I = 1/2$ π-N scattering length for $K = 0.1665$.

To summarize, we have explored the possibility of extracting the N-N scattering lengths from numerical simulations of lattice QCD. Albeit carried out at heavy quarks, our results show that the attractive forces work in both channels of s-wave N-N scattering, its scattering

lengths being significantly larger compared to the π-N and π-π scattering lengths. It remains an important and realistic problem to confirm that reducing the quark mass results in an increase of scattering lengths to the values observed experimentally. Such a calculation, however, requires a much larger lattice and smaller quark masses than are possible at present and, hence, has to await a development of the computing power. In the mean time a possible analytical approach would be to develop effective theories for the nuclear force for a heavy quark to interpolate our lattice results to the effective low energy theory with realistic quark masses, as has been done for the mesonic sector with the aid of the chiral Lagrangian formalism.

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[8] This is different from the cases of π-π and π-N; their dominant low energy force arises from the exchange of a ρ meson, whose mass, in contrast to the π meson mass, does not differ radically from the realistic value even for heavy quarks. For N-N scattering an approximate degeneracy of pseudoscalar and vector meson masses for heavy quarks should lead to a substantial cancellation between the attractive pseudoscalar exchange and the repulsive vector meson exchange.