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Using all-to-all propagators for $K \to \pi\pi$ decays

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In order to determine the direct CP-violation parameter ε' from first principles, the decay amplitude for $K \to \pi\pi(\Delta I = 1/2)$ must be calculated on the lattice, where the main difficulty is the disconnected diagrams appearing in the correlation function. In order to control the statistical fluctuations in these disconnected diagrams, we will use all-to-all propagators, which allow the construction of $\pi\pi$ operators with reduced coupling to vacuum. The resulting I=0 $\pi\pi$ scattering phase shift obtained using this methods shows that it works as we expected. We will also describe the current progress in implementing this method for $K \to \pi\pi$ decays.

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1. Motivations of using all-to-all propagator

The measure of direct CP-violation (in $K \to \pi\pi$) is determined by:

$$\varepsilon' = \frac{ie^{i(\delta_2-\delta_0)}}{\sqrt{2}} \frac{ReA_2}{ReA_0}\left(\frac{ImA_2}{ReA_2} - \frac{ImA_0}{ReA_0}\right) , \quad (1.1)$$

where δ_2 and δ_0 are the strong phase shifts from $\pi\pi$ scattering, A_2 and A_0 are the two decay amplitudes. A_2 is now calculated with physical kinematics and physical quark mass[1]. The only thing left is the physical A_0. The traditional way of calculating A_0 is by using a wall-source-wall-sink approach, where the quark operators are distributed in the whole 3D space. The π and K wave functions constructed in this way are usually bigger than their actual size, which leads to unphysical contribution to the resulting amplitude. For the A_0 calculation, when using the wall-source-wall-sink approach, the coupling between the two-pion operator and the vacuum will receive contributions from propagators that go from 3D-volume to 3D-volume, which results in a larger coupling to the vacuum state than if we have localised π and K operators.

Figure 1: Left: Using wall-source-wall-sink propagator. Right: Using all-to-all method

The all-to-all propagator method allows us to calculate the quark propagator from arbitrary source point to arbitrary sink point, so we can certainly make the meson operators smaller. As figure 1 shows, all-to-all propagators allows us to control the size of mesons, giving better overlap with ground state and smaller overlap with vacuum. (This figure also shows an already recognized method [4] for substantially reducing the error coming from the vacuum state: putting the source for each pion on a different time slice.)

2. Description of all-to-all propagator

The unit matrix can always be approximated by the outer product of some random vectors:

$$I \approx \sum_{1}^{N} \eta_j \eta_j^\dagger \quad (2.1)$$

The larger N is, the better approximation it is. Using this idea, the inverse of Dirac operator can be approximated as[3, 2]:

$$D^{-1} \approx \sum_{i}^{N_{ev}} \frac{h_i h_i^\dagger}{\lambda_i} + \sum_{j}^{N_{hit}} (D^{-1}_{deflate}\eta_j)\eta_j^\dagger \quad (2.2)$$

N_{ev} is the number of low eigen-modes, N_{hit} is the number of random vectors. They could both be adjusted depending on the quark mass. For simplicity, we will call the fermion vectors in the set $\{\frac{h_i}{\lambda_i}, D^{-1}_{deflate}\eta_j\}$ as v, call those in the set $\{h^\dagger_i, \eta^\dagger_j\}$ as $w^\dagger$. Both v and $w^\dagger$ carry indices of mode number and space-time-spin-color. Now the propagator between two arbitrary points can be written as:

$$D^{-1}_{x,a,\alpha;y,b,\beta} = \sum_{i=1}^{N_{ev}+N_{hit}} v^i_{x,a,\alpha} {w^i}^\dagger_{y,b,\beta} \tag{2.3}$$

Here the x and y are space-time indices,α and β are spin indices, a and b are color indices, we will keep the same convention though out this proceeding. Once we have calculated the v vectors and w vectors, we can construct the correlation functions as we want. As an example, the pseudo-scaler, point-source, point-sink, two point function is written as:

$$\begin{aligned}\sum_{x,y} D^{-1}_{x,a,\alpha;y,b,\beta}(\gamma_5)_{\beta\gamma} D^{-1}_{y,b,\gamma;x,a,\sigma}(\gamma_5)_{\sigma\alpha} &= \sum_{x,y,i,j}(v^i_{x,a,\alpha}{w^i}^\dagger_{y,b,\beta})(\gamma_5)_{\beta\gamma}(v^j_{y,b,\gamma}{w^j}^\dagger_{x,a,\sigma})(\gamma_5)_{\sigma\alpha} \\ &= \sum_{i,j}(\sum_x ({w^j_{x,a,\sigma}}^\dagger(\gamma_5)_{\sigma\alpha}v^i_{x,a,\alpha})\sum_y({w^i}^\dagger_{y,b,\beta}(\gamma_5)_{\beta\gamma}v^j_{y,b,\gamma})) \\ &= \sum_{i,j}\pi^{ji}_{t_x}\pi^{ij}_{t_y}\end{aligned} \tag{2.4}$$

Repeated indices are summed, and the summation on x and y is over their spacial indices, leaving the correlator as a function of time.

A less trivial example is one of the $K \to \pi\pi$ contractions:

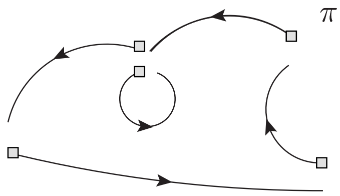

Figure 2: One of the $K \to \pi\pi$ contractions. In the middle is a four-quark operator ($\Delta S = 1$), shaded boxes are where the random sources have been used.

$$\begin{aligned}C(t_K,t_\pi,t_{\pi'},x_{op}) &= \sum_{\vec{x}_{op}} Tr\{\gamma_\mu(1-\gamma_5)L(\vec{x}_{op},t_{op};t_\pi)\gamma_5 L_w(t_\pi;t_{\pi'})\gamma_5 L_w(t_{\pi'};t_K)\gamma_5 S(t_K;\vec{x}_{op},t_{op})\} \\ &\quad \cdot Tr\{\gamma^\mu(1-\gamma_5)L(\vec{x}_{op},t_{op};\vec{x}_{op},t_{op})\} \\ &= \sum_{\vec{x}_{op}}\{{w'^m}^\dagger_{x_{op},a,\alpha}(\gamma_\mu(1-\gamma_5))_{\alpha\alpha}v^i_{x_{op},a,\alpha}\}\cdot\{{w^j}^\dagger_{x_{op},b,\beta}(\gamma^\mu(1-\gamma_5))_{\beta\beta}v^j_{x_{op},b,\beta}\} \\ &\quad \cdot\pi^{ik}_{t_\pi}\pi^{kl}_{t'_\pi}K^{lm}_{t_K}\end{aligned} \tag{2.5}$$

On the first line of (2.5), L is the propagator for the up or down quark, S is the propagator for the strange quark. In the last step, the summation is over spacial components of $\vec{x}_{op}$.

3. Choosing the meson field wave function

The meson operator in (2.4) is actually a point-like meson, in which the two quarks are right on top of each other. A physical meson should have a finite size. In order to make a better overlap with the ground state, we can allow some displacement between the two quarks, link them by Coulomb fixed gauge $S_a(x)$, and weight the operator by a meson field wave function $\phi(r)$:

$$\pi^{ij}_{t_x} = \sum_{x,x',a,b,c,\alpha,\beta} w^{i\dagger}_{x,a,\alpha} S^{\dagger}_{ab}(x)(\gamma_5)_{\alpha\beta} S_{bc}(x') v^{j}_{x',c,\beta} \phi(|x-x'|) \tag{3.1}$$

The trivial wave function $\phi(r) = 1$ corresponds to the wall-source-wall-sink approach. A better choice is a localized wave function, for example:

$$\phi(|x-x'|) = e^{-|x-x'|/r} \tag{3.2}$$

The parameter r controls the size, and it needs to be tuned until the meson has good overlap with its ground state while the two-meson state still has a relatively small overlap with vacuum. We did a lot of tests on a $16^3 \times 32$ lattice, with 2+1 domain wall fermion and Iwasaki gauge action. The lattice spacing is $a^{-1} = 1.732GeV$, pion and kaon masses are $m_\pi = 422MeV, m_K = 766MeV$. Figure (3) shows that the size of the meson field do affect the plateau and error bar. As we make the

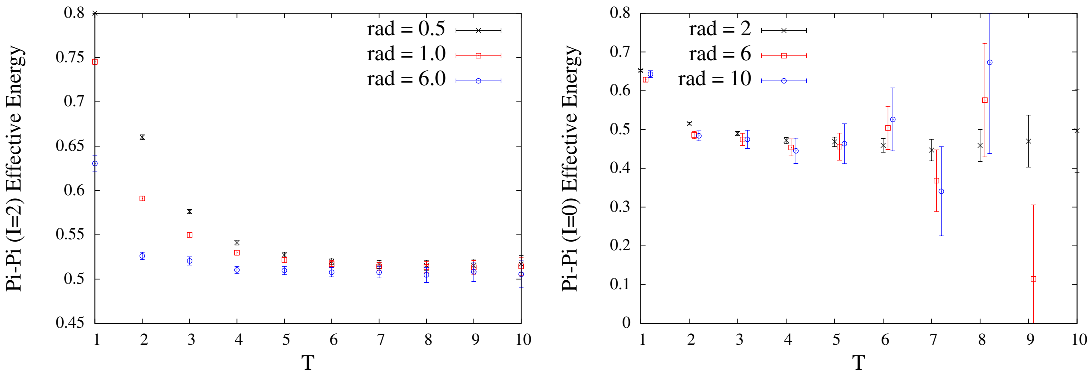

Figure 3: Effective mass plot for I=2 and I=0 pi-pi scattering, using meson field wave function in (3.2) with different size r

radius smaller, the (I=2) pi-pi plateau starts at later time, showing the pi-pi state has poorer overlap with its ground state; on the other hand, if we make the radius bigger, the coupling of pi-pi state to vacuum grows and the (I=0) pi-pi plateau becomes significantly noisier. So there is an optimal choice of the meson size, which should corresponds to its physical size. In our measurement, we find $r = 2$ gives almost the best results.

4. Deal with the four-quark operator

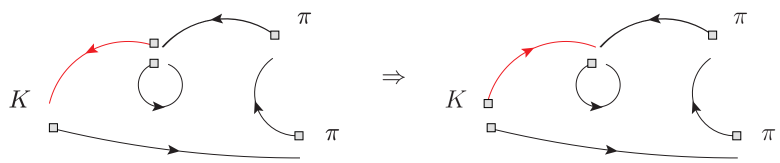

Figure 4: Left: original contraction. Right: a better way to do contraction.

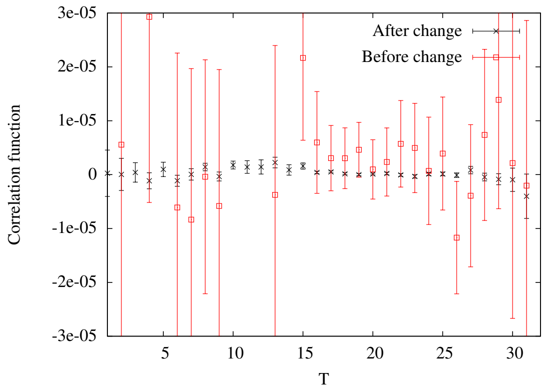

Figure 5: Measured correlation function corresponds to Figure 4

When using all-to-all propagators to calculate the $K \to \pi\pi$ decay amplitude, it matters where we put the random numbers (Because of γ_5-hermiticity, we can choose which end is the source and which end is the sink for each propagator). Figure 4 shows two ways of doing the contraction, shaded boxes are where we have used random numbers. The left panel in Figure 4 shows what we originally used to calculate the correlation function, right panel shows a much better way. The lesson is that when using all-to-all propagators it is best to locate as few random sources as possible at the four-quark operator. Figure 5 shows how large the improvement is. The lattice setup is the same as in section 3. 100 low eigen-modes are used for the light quark propagator.

5. Conclusion

We calculated (I=0) pi-pi phase shift using both the wall-source-wall-sink propagators and all-to-all propagators using a meson wave function with radius 2. We compare them using the same 200 configurations. The result indicates that all-to-all propagator gives at least two times smaller error bar.

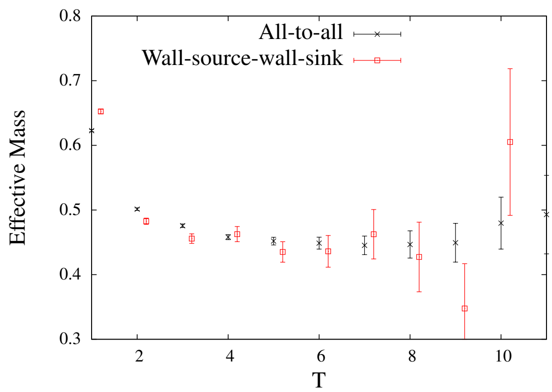

Figure 6: (I=0) pi-pi effective energy

	$E_{\pi\pi}^{I=0}$
All-to-all	0.449(10)
Wall-source-wall-sink	0.438(25)

Table 1: (I=0) pi-pi effective energy

For the $(\Delta I = 1/2)K \to \pi\pi$ decay,we also compared these two approaches, contribution from each operator are listed in table 2.

	Wall-source-wall-sink(200 conf)		All-to-all(200 conf)	
i	$Re(A_0)(GeV)$	$Im(A_0)(GeV)$	$Re(A_0)(GeV)$	$Im(A_0)(GeV)$
1	2.6(97)e-08	0	3.8(33)e-08	0
2	4.8(17)e-07	0	2.1(15)e-07	0
3	-2.0(21)e-09	1.1(11)e-11	4.3(74)e-10	2.4(41)e-12
4	1.35(70)e-08	-4.4(23)e-11	1.6(33)e-09	5(11)e-12
5	-1.2(82)e-10	-6(43)e-13	4.7(29)e-10	2.4(15)e-12
6	-1.41(66)e-08	-8.5(40)e-11	-1.27(29)e-08	-7.6(18)e-11
7	7.0(22)e-11	1.18(36)e-13	8.11(75)e-11	1.36(13)e-13
8	-4.83(78)e-10	-2.35(38)e-12	-4.41(38)e-10	-2.15(19)e-12
9	-4.9(25)e-14	-3.2(16)e-13	9(10)e-15	-6.0(67)e-13
10	-2(17)e-12	0.6(40)e-13	1.46(68)e-11	-3.5(16)e-13
Total	5.1(16)e-07	-5.8(41)e-11	2.4(16)e-07	-6.9(22)e-11

Table 2: $\Delta I = 1/2$ physical amplitude

Although the total real part doesn't show a significant improvement, the total imaginary part goes down by roughly a factor of 2, and almost every operator has smaller error bar.

	Wall-source-wall-sink	All-to-all	All-to-all fully parallelized (expected)
Time	40m	70m	50m

Table 3: Computation cost

These measurements are all done on an IBM BG/Q 128-node machine, the computation cost increases by about 25% when using all-to-all propagator. So we still have a gain in efficiency and the all-to-all propagator is helpful in suppressing the fluctuation in disconnected diagrams, for both I=0 pi-pi phase shift and $\Delta I = 1/2$ $K \to \pi\pi$.

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