Supplemental Material: Improved Hamiltonians for Quantum Simulations

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DERIVATION FOR THE IMPROVED POTENTIAL TERM

The classical errors of V_{KS} can be analyzed via the series expansion of the one-plaquette Wilson loop

$$\mathrm{Re}\,\mathrm{Tr}\,P_{ij}(x) = \mathrm{Re}\,\mathrm{Tr}\,\mathbf{P}\{e^{ig_s\oint_{1\times1}A\cdot dx}\}, \tag{1}$$

where $\mathbf{P}$ stands for the path-ordering. To do this, we transform the line integral of A into the surface integral ds_{ij} with Stokes theorem, and then Taylor expand it around the center of the plaquette $\mathbf{x}_c$ to the next leading order:

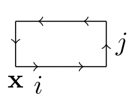
$$\begin{aligned}\oint_{1\times1} dx\cdot A &= \int_{-a/2}^{a/2}\int_{-a/2}^{a/2} ds_{ij}F_{ij}(\mathbf{x}_c+\mathbf{x}')\\ &= a^2F_{ij}(\mathbf{x}_c) + \frac{a^4}{24}(D_i^2+D_j^2)F_{ij}(\mathbf{x}_c) + O(a^6).\end{aligned} \tag{2}$$

We then obtain

$$\begin{aligned}\mathrm{Re}\,\mathrm{Tr}\,P_{ij}(\mathbf{x}) = \mathbb{1} - g_s^2a^4\,\mathrm{Tr}\Big[\frac{1}{2}F_{ij}^2(\mathbf{x}_c)\\ + \frac{a^2}{24}F_{ij}(\mathbf{x}_c)(D_i^2+D_j^2)F_{ij}(\mathbf{x}_c) + \mathcal{O}(a^4)\Big] + \mathcal{O}(g_s^4).\end{aligned} \tag{3}$$

The $\mathcal{O}(a^2)$ errors can be canceled by including gauge invariant two-plaquette Wilson loops in the potential:

$$\mathrm{Re}\,\mathrm{Tr}\,R_{ij}(\mathbf{x}) = \mathrm{Re}\,\mathrm{Tr}\left\{\quad\right\}. \tag{4}$$



At classical level, we can ignore the bent diagram. The improved potential can be written as V_I:

$$V_I = -\frac{2}{ag_s^2}\sum_{\mathbf{x},i<j}\mathrm{Re}\,\mathrm{Tr}\left[\beta_{V0}P_{ij}(\mathbf{x}) + \beta_{V1}\left(R_{ij}(\mathbf{x})+R_{ji}(\mathbf{x})\right)\right], \tag{5}$$

with the coefficients β_{V0} and β_{V1} being carefully chosen to cancel the classical $\mathcal{O}(a^2)$ errors. Following the same procedure as in Eq. (3), we obtain the lowest order terms of R_{ij}:

$$\begin{aligned}\mathrm{Re}\,\mathrm{Tr}\,R_{ij}(\mathbf{x}) = 1 - g_s^2a^4\,\mathrm{Tr}\Big[2F_{ij}^2(\mathbf{x}_c)\\ + \frac{a^2}{6}F_{ij}(\mathbf{x}_c)(4D_i^2+D_j^2)F_{ij}(\mathbf{x}_c) + \mathcal{O}(a^4)\Big] + \mathcal{O}(g_s^4).\end{aligned} \tag{6}$$

Substituting Eq. (3) and Eq. (6) into Eq. (5) and requiring no classical $\mathcal{O}(a^2)$ errors to the leading-order terms such that

$$V_I = a^3\left(\sum_{\mathbf{x}_c,i<j}\mathrm{Tr}\,F_{ij}^2(\mathbf{x}_c) + \mathcal{O}(a^4)\right) + \text{constant}, \tag{7}$$

one obtains $\beta_{V0} = \frac{5}{3}, \beta_{V1} = -\frac{1}{12}$.

LEFT AND RIGHT ELECTRIC FIELD OPERATORS

We present a brief review of the properties of left and right electric field operators based on the discussion in [1]. $\hat{L}_i(\mathbf{x}) = \hat{L}_i^a(\mathbf{x})\lambda_a$ is the left electric field operator satisfying the following commutation relations [1, 2][1]:

$$[\hat{L}_i^a(\mathbf{x}), \hat{U}_i(\mathbf{x})] = \lambda_a\hat{U}_i(\mathbf{x}), \tag{8}$$

$$[\hat{L}_i^a(\mathbf{x}), \hat{L}_i^b(\mathbf{x})] = -if_{abc}\hat{L}_i^c(\mathbf{x}), \tag{9}$$

where $\{\lambda_a\}$ are the group's generators and f_{abc} are the structure constants.

The $\hat{R}_i(\mathbf{x})$ operator defined in the main text:

$$\hat{R}_i(\mathbf{x}) \equiv \hat{U}_i^\dagger(\mathbf{x})\hat{L}_i(x)\hat{U}_i(\mathbf{x}) = \hat{R}_i^a(\mathbf{x})\lambda_a, \tag{10}$$

corresponds to the right electric field operator obeying the following commutation relations: [1]

$$[\hat{R}_i^a(\mathbf{x}), \hat{U}_i(\mathbf{x})] = \hat{U}_i(\mathbf{x})\lambda_a, \tag{11}$$

$$[\hat{R}_i^a(\mathbf{x}), \hat{R}_i^b(\mathbf{x})] = if_{abc}\hat{R}_i^c(\mathbf{x}), \tag{12}$$

$$[\hat{L}_i^a(\mathbf{x}), \hat{R}_i^b(\mathbf{x})] = 0. \tag{13}$$

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[1] Our definition of $\hat{L}$ differs from [2] by a minus sign.

For the following discussions, we will neglect the position dependence on $\mathbf{x}$ and the subscript i of operators for simplicity. $\hat{L}(\hat{R})$ transforms $\hat{U}$ operators as follows [2]:

$$e^{i\alpha_a \hat{L}^a} \hat{U}_{mn} e^{-i\alpha_a \hat{L}^a} = U_{mk}(\alpha) \hat{U}_{kn}, \tag{14}$$
$$e^{i\alpha_a \hat{R}^a} \hat{U}_{mn} e^{-i\alpha_a \hat{R}^a} = \hat{U}_{mk} U_{kn}(\alpha), \tag{15}$$

with matrix-valued $U(\alpha) = e^{i\alpha^b \lambda_b}$. And $|U\rangle$ transforms under $e^{-i\alpha_a \hat{L}^a}$ and $e^{-i\alpha_a \hat{R}^a}$ as

$$\begin{aligned} e^{-i\alpha_a \hat{L}^a} |U\rangle &= |U(\alpha) \cdot U\rangle, \\ e^{-i\alpha_a \hat{R}^a} |U\rangle &= |U \cdot U(\alpha)\rangle. \end{aligned} \tag{16}$$

KINETIC TERM CIRCUIT DERIVATION

First, we prove that the circuit $\mathcal{U}_{K_{2L}} \equiv e^{i\theta \operatorname{Tr}(\hat{L}_2 - \hat{R}_1)^2}$ commutes with $\hat{U}_1 \hat{U}_2$ by calculating the following commutator:

$$\begin{aligned} &[(\hat{L}_2^a - \hat{R}_1^a), (\hat{U}_1 \hat{U}_2)_{ij}] \\ =&(\hat{U}_1)_{ik} [\hat{L}_2^a, (\hat{U}_2)_{kj}] - [\hat{R}_1^a, (\hat{U}_1)_{ik}] (\hat{U}_2)_{kj} \\ =&(\hat{U}_1)_{ik} (\lambda^a)_{kl} (\hat{U}_2)_{lj} - (\hat{U}_1)_{il} (\lambda^a)_{lk} (\hat{U}_2)_{kj} \\ =&\ 0. \end{aligned} \tag{17}$$

This subsequently leads to $[\mathcal{U}_{K_{2L}}, (\hat{U}_1 \hat{U}_2)] = 0$. The time evolution circuit for the two-link term $\mathcal{U}_{K_{2L}}$ thus preserves the product of $U_1 U_2$ and can be written as:

$$\langle U_1', U_2' | \mathcal{U}_{K_{2L}} | U_1, U_2 \rangle = \delta_{U_1' U_2', U_1 U_2} \mathcal{A}(U_1, U_2, U_1'). \tag{18}$$

We obtain $\mathcal{A}(U_1, U_2, U_1')$ by integrating over U_2' on both sides of Eq. (26), cancelling $\delta_{U_1' U_2', U_1 U_2}$:

$$\mathcal{A}(U_1, U_2, U_1') = \int dU_2' \langle U_1', U_2' | \mathcal{U}_{K_{2L}} | U_1, U_2 \rangle. \tag{19}$$

Define the change from U_2 to U_2' as $V \equiv U_2' U_2^{-1}$, which is evidently a group element and can be parameterized as $V = e^{i\alpha^b \lambda_b}$. Thereby the operator $e^{i\alpha_a \hat{L}_2^a}$ generates the transformation from $\langle U_2|$ to $\langle V U_2| = \langle U_2'|$. Thus, the final state can be written as

$$\langle U_1', U_2'| = \langle U_1', V U_2| = \langle U_1', U_2| \, e^{i\alpha_c \hat{L}_2^c}. \tag{20}$$

As the Haar measure is invariant under product with any group element, we have

$$dU_2' = d(V U_2) = dV. \tag{21}$$

Replacing $\langle U_1', U_2|$ and dU_2' in the RHS of Eq. (19) with Eq. (20) and Eq. (21), we get:

$$\mathcal{A}(U_1, U_2, U_1') = \int dV \, \langle U_1', U_2| \, e^{i\alpha_c \hat{L}_2^c} \mathcal{U}_{K_{2L}} | U_1, U_2 \rangle. \tag{22}$$

The integral over all group transformations $\int dV e^{i\alpha_c \hat{L}_2^c}$ is equivalent to projecting the $|U_2\rangle$ register to the ground state of $\hat{L}_2^2$ ($|J_2 = 0\rangle$) up to a normalization factor fixed to be consistent with $\int dV = |G|$ [3]. This can be easily understood as follows. Any generator $\hat{L}^b$ annihilates the state $\int dV e^{i\alpha_a \hat{L}^a} |U\rangle$ for arbitrary $|U\rangle$, as a result of Stokes' theorem on a compact manifold:

$$\hat{L}^b \int dV e^{i\alpha_a \hat{L}^a} |U\rangle = -i \int dV \frac{\partial}{\partial \alpha_b} e^{i\alpha_a \hat{L}^a} |U\rangle = 0. \tag{23}$$

Therefore, $\int dV e^{i\alpha_a \hat{L}_2^a} |U\rangle \propto |J_2 = 0\rangle$ and we get the following:

$$\int dV e^{i\alpha_a \hat{L}_2^a} = |G| \, |J_2 = 0\rangle \langle J_2 = 0| = |G| \hat{P}_{J_2 = 0}. \tag{24}$$

Substitute Eq. (24) into Eq. (22) and notice that, as $\mathcal{U}_{K_{2L}}$ commutes with $\hat{R}_2^2$, it conserves the quantum number J_2, and therefore, $\hat{P}_{J_2=0} \, \mathcal{U}_{K_{2L}} = \hat{P}_{J_2=0} \, \mathcal{U}_{K_{2L}} \, \hat{P}_{J_2=0}$. Insert another $\hat{P}_{J_2=0}$ after $\mathcal{U}_{K_{2L}}$ in Eq. (22) and we find $\mathcal{A}$ is:

$$\begin{aligned} \mathcal{A}(U_1, U_2, U_1') &= \langle U_1', J_2 = 0| \mathcal{U}_{K_{2L}} |U_1, J_2 = 0\rangle \\ &= \langle U_1'| \, e^{i\theta \operatorname{Tr} \hat{R}_1^2} |U_1\rangle, \end{aligned} \tag{25}$$

which gives

$$\langle U_1', U_2' | \mathcal{U}_{K_{2L}} | U_1, U_2 \rangle = \delta_{U_1' U_2', U_1 U_2} \langle U_1' | \, e^{i\theta \operatorname{Tr} \hat{L}_1^2} |U_1\rangle. \tag{26}$$

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