

SUPPLEMENTARY INFORMATION:

Towards determining the (2+1)-dimensional Quantum Electrodynamics running coupling with Monte Carlo and quantum computing methods

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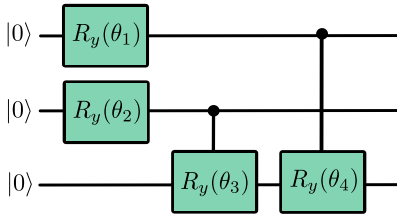
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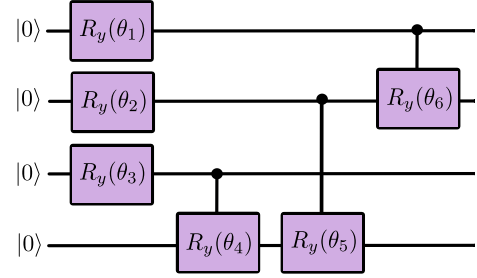
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I. SUPPLEMENTARY NOTE 1: GRAY ENCODING VARIATIONAL CIRCUITS

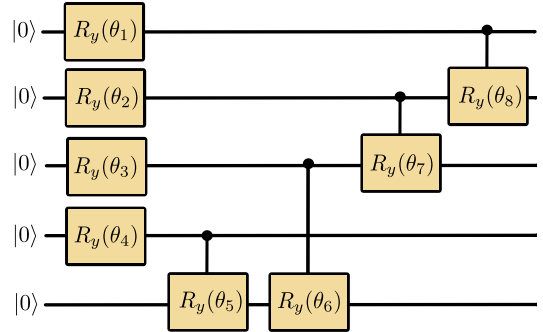
As outlined in the Section “Numerical setup for quantum computation”, the qubit requirements for the adopted encoding follow a logarithmic scaling. Specifically, for certain values of l , the exclusion of a single state suffices and as a consequence, the complexity of the required gate set for circuit implementation is significantly reduced. The logic of the exclusion of states outside the reduced Hilbert space $\mathcal{H}_{2l+1}$ for $l > 1$ mirrors that of the $l = 1$ case. Moreover, when only one state requires exclusion, a discernible pattern emerges in the gate structure. In this section, we present the variational circuits corresponding to $l = 3, 7, 15$, in Supplementary Figs. 1, 2, 3 respectively.



Supplementary Fig. 1: **Variational circuit for Gray encoding with low truncation.** The circuit corresponds to truncation $l = 3$. $|010\rangle$ represents the *vacuum state* and the state $|100\rangle$ excluded.



Supplementary Fig. 2: **Variational circuit for Gray encoding with medium truncation.** The circuit corresponds to truncation $l = 7$. $|0100\rangle$ represents the *vacuum state* and the state $|1000\rangle$ excluded.



Supplementary Fig. 3: **Variational circuit for Gray encoding with high truncation.** The variational circuit describes circuit $l = 15$. $|01000\rangle$ represents the *vacuum state* and the state $|10000\rangle$ excluded.

The next step is to establish an appropriate pattern for entangling multiple gauge fields. This task is particularly important when working with an electric (magnetic) basis formulation, especially in regimes characterized by weak (strong) coupling. In this paper, we devised a struc-

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ture capable of entangling all gauge fields, while guaranteeing the exclusion of unphysical states, as depicted in the example of Supplementary Fig 4.

We remark that integrating Gauss's law a priori makes the Hamiltonian non-local, and hence requires more gates per qubit. See e.g. Ref [1] for a discussion on the effect on a real noisy quantum device. In this work, the noise is purely statistical, as we simulate classically the behavior of a quantum device. In the future, our work will be devoted to exploring more resource-efficient alternatives. This will involve an analysis of an efficient mapping of the square lattice structure to quantum devices with limited connectivity.

II. SUPPLEMENTARY NOTE 2: ΔE

In this section, we report our investigation of the mass gap ΔE with Monte Carlo simulations. We find numerical evidence that the volume $L/a = 3$ used with the present Hamiltonian formulation is too small to match the mass gap of the theory. Nonetheless, we provide some quantitative estimate of the coupling range needed for this approach, finding that a slight increase in the volume size on the Hamiltonian simulations would allow for such a matching procedure.

A $U(1)$ gauge theory in $(2+1)$ -dimensions is a non-trivial theory only at finite lattice spacing, where it can be approximated by a plasma of magnetic monopoles in an external field [2]. It has been shown that the theoretical prediction for the gauge coupling dependence of the mass gap is in agreement also with numerical determinations [3]. In the continuum limit, the theory becomes equivalent to a free massive scalar theory [4], whose lightest state is the analogue of a “massive photon”. At finite lattice spacing, this is found to be a glueball, with $J^{PC} = 0^{--}$ quantum numbers [5–8]. The wavefunction of the 0^{--} state can be interpolated by the operator [9]:

$$\hat{\phi}(t) = \frac{1}{V} \sum_{\mathbf{r}} \text{Im Tr} \left[\hat{P}(t, \mathbf{r}) - \hat{P}^\dagger(t, \mathbf{r}) \right]. \quad (1)$$

The sum over the spatial coordinates $\mathbf{r}$ ensures the particle is at rest. In a Monte Carlo simulation with time extent T we can find the mass gap from the expectation value (over the gauge configurations) of the following correlation function [10],

$$C_T(t) = \langle \hat{\phi}(t) \hat{\phi}(0) \rangle_T. \quad (2)$$

We note that $\hat{\phi}$ is hermitian by construction. According to its spectral decomposition, for large values of t the above correlator approaches the expression:

$$C_T(t) \rightarrow |\langle 0^{--} | \hat{\phi}(0) | 0 \rangle|^2 \left(e^{-Mt} + e^{-M(T-t)} \right), \quad (3)$$

where $|0\rangle$ is the interacting vacuum and we have taken into account also the backward signal from $T-t$. M is the

mass of the lightest state interpolated by the operator $\hat{\phi}$. For each ensemble, i.e. volume and coupling constant, we compute the following effective mass curve for the 0^{--} correlator from the following implicit expression,

$$\frac{C(t)}{C(t+1)} = \frac{\cosh(M_{\text{eff}}(t) \cdot (t - T/2))}{\cosh(M_{\text{eff}}(t) \cdot (t + 1 - T/2))}. \quad (4)$$

Namely, for each t the value $M_{\text{eff}}(t)$ is found by numerically solving Eq. (4). Finally, we consider the time interval where $M_{\text{eff}}(t)$ plateaus within the statistical uncertainty, and fit it to a constant value.

We have performed Monte Carlo simulations in the range $1.35 \leq \beta \leq 2.25$ and $6 \leq L/a \leq 16$. In our setup $T/a = 16$ for all the ensembles. We have checked that this value of the time extent is compatible with the infinite time extent limit within the uncertainty. Similarly, we have verified that in this range of β , the values at $L/a = 16$ are compatible with their infinite volume limit.

The gauge field configurations have been produced using the Hybrid Monte Carlo (HMC) algorithm (see Ref. [11]). The effects of autocorrelation have been taken into account with the method of Ref. [12] in order to correctly estimate the uncertainty on the data.

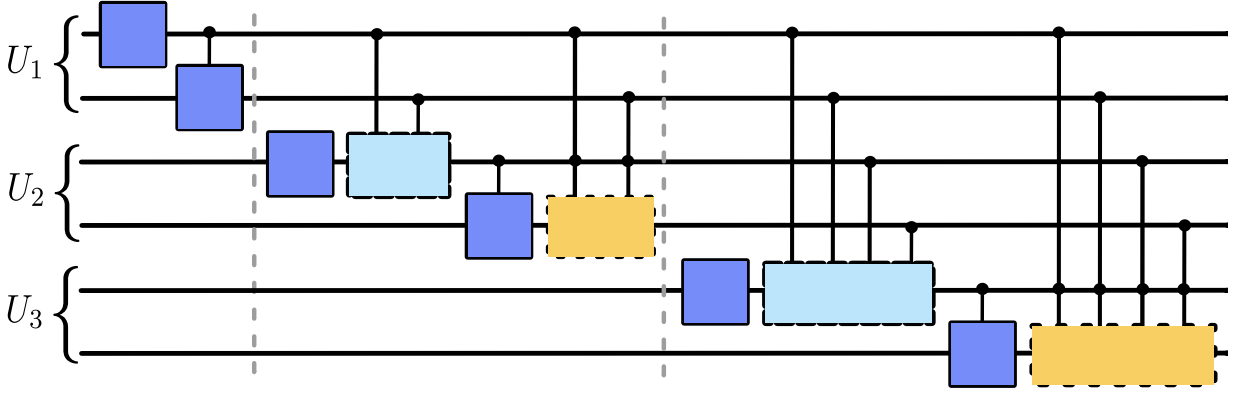
We recall that ultimately our goal consists of matching the Lagrangian and Hamiltonian results, with the latter being limited to $L/a = 3$. A direct evaluation of the mass gap from euclidean correlators at this volume is challenging, as the excited states contamination becomes significant and the signal-to-noise-ratio of the correlator becomes poor. Therefore, we are interested in the small volume extrapolations.

In Supplementary Fig. 5, we show the β dependence of the mass of the glueball 0^{--} , while in Supplementary Fig. 6 we show the volume dependence of the latter. Finite Volume Effects (FVEs) are fitted according to the following Ansatz inspired by QCD [13]:

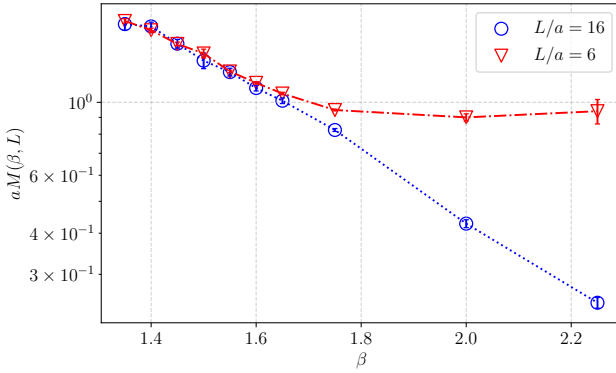
$$M(L) = M(L = 16a) \left[1 + c \cdot \frac{e^{-\frac{\sqrt{3}}{2} M(L=16a) \cdot L}}{M(L = 16a) \cdot L} \right], \quad (5)$$

where we consider the values at $L = 16a$ as an approximation of the ones at $L = \infty$, and c is a free parameter of the fit.

Looking at the data, we can make the following considerations. For large β we have a smaller lattice spacing, and hence smaller volume in physical units. As the volume is reduced to $L/a = 3$, the Compton wavelength of the glueball does not fit the lattice, and we cannot interpret the result as the mass of a particle. Moreover, FVEs are not under control in this region, unless the lattice spacing becomes coarse. At small β , the lattice is coarse enough to make the glueball fit, though several values of β give values above the cutoff. According to our results, we conclude that the “sweet spot” to perform matching using the glueball mass would be around $\beta \approx 1.8$, and with a Hamiltonian with at least $(L/a) \geq 6$. It is understood that this value of the coupling should

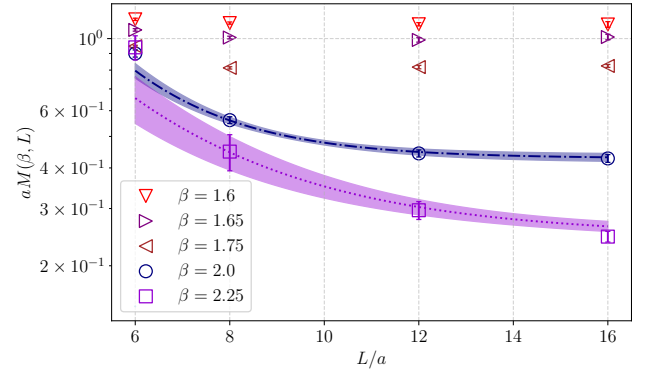


Supplementary Fig. 4: **Generalization of the Gray circuit for three gauge fields.** Circuit acting on the links U_1, U_2, U_3 and at truncation $l = 1$. The circuit starts at U_1 with the gates of the Gray structure (blue solid boxes) as in Fig. 10 of the main manuscript. The second gauge field U_2 has a R_y gate in the first qubit, which is also entangled to U_1 with a Control- R_y gate (lightblue dashed box), for compactness represented with a single box and two vertical lines. To entangle the second qubit of U_2 we include two Multicontrol- R_y gates (orange dotted box). The procedure is similar for U_3 , which is now entangled to U_1 and U_2 . With this structure we respect the subset of physical states for truncation $l = 1$ and entangle the gauge fields of the system.



Supplementary Fig. 5: **Coupling dependence of the lowest-lying glueball mass.** Dependence of the glueball mass with quantum numbers $J^{PC} = 0^{--}$ on β . The red dashed and blue dotted lines correspond respectively to the values $L/a = 6, 16$. The temporal extent is $T/a = 16$ for all points.

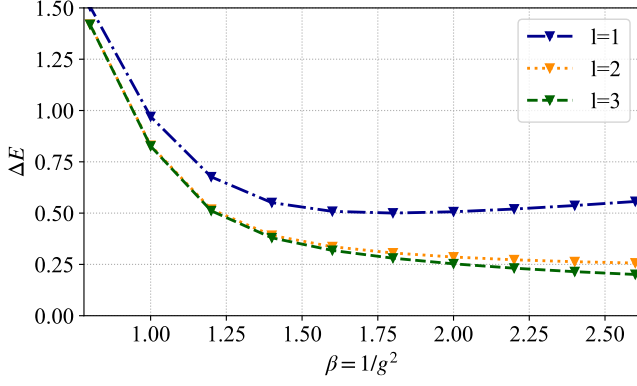
be extrapolated to the Hamiltonian limit [14] in order to compare the two formalisms. We leave this type of analysis to future work. The steps to match the Hamiltonian to the Lagrangian formulation shall be the same as for the plaquette expectation value, as described in the Section “Matching strategy for 3×3 PBC system”, but applied to the mass gap. We remark that at the moment we have computed the mass gap in the Hamiltonian formulation with truncations $l \in [1, 3]$ by using exact diagonalization, as illustrated in Supplementary Fig. 7. The missing part is the Hamiltonian limit of β_{MC} and the glueball mass.



Supplementary Fig. 6: **Volume dependence of the lowest-lying glueball mass.** Mass of the glueball mass with quantum numbers $J^{PC} = 0^{--}$ as a function of the volume. Different markers correspond to different values of β , as specified in the legend. The plot is limited to the values of $\beta \geq 1.6$ for better visualization of FVEs. The fit from Eq. (5) for the two highest values of β and $L/a \geq 8$ is shown explicitly.

III. SUPPLEMENTARY NOTE 3: ELECTRIC/MAGNETIC BASIS ANALYSIS

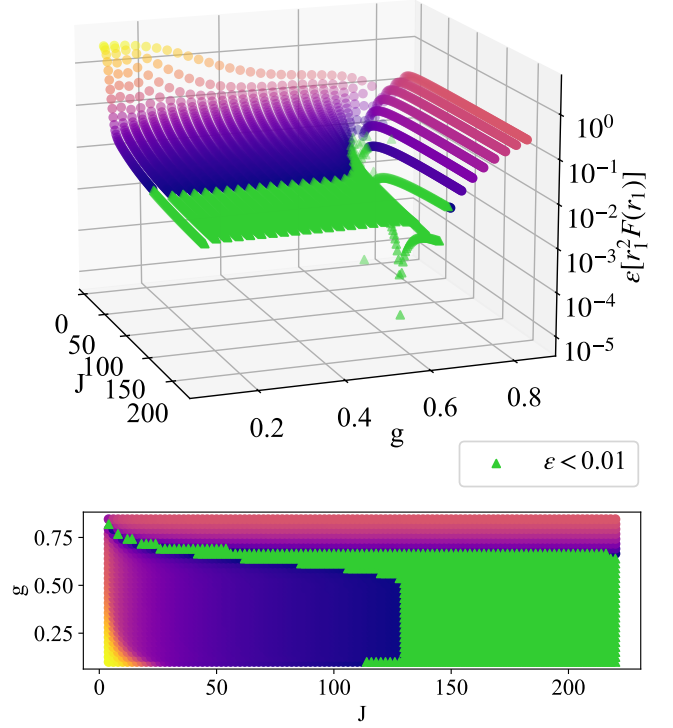
In this section, we extend the analysis for the step scaling method of the Section “Step scaling approach”, with an inclusion of both electric and magnetic basis. We start from the value of $\beta \equiv \beta_{MC}$ where we match with Monte Carlo, and we compute the values of the two static forces both in the electric and magnetic basis, within a range of truncations. For small β (large g) the electric basis is



Supplementary Fig. 7: **Energy gap from exact diagonalization.** Energy gap of the theory for a 3×3 PBC system obtained with exact diagonalization at truncations $l \in [1, 3]$.

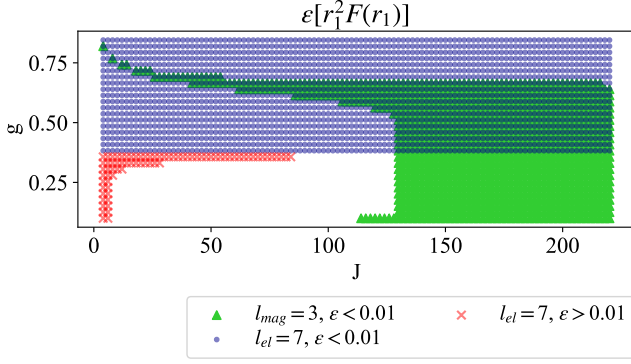
preferable, as the electric Hamiltonian (see Eq. (2) in the main text) is dominant and we do not need a large value of l . We decided to consider $l = 7$, both to have good precision in the results, but also because with a Gray-type encoding (see the Section “Numerical setup for quantum computation” in the main text and Section [Supplementary Note 1: Gray encoding variational circuits](#)), we can exploit a limited number of qubits for a higher number of states. We also use a larger truncation in the electric basis, i.e. $l = 32$, to have a reference value for comparison with the magnetic basis, in fact with this high truncation the results are more likely independent of l and have a physical meaning. The value is chosen by testing the convergence of l up to a precision where the absolute error between the results with l and $l - 1$ is $\mathcal{O}(10^{-5})$ or lower. For the magnetic basis, we also fix $l = 7$ and scan over the discretization parameter J , to find a good approximation of the previous reference value. We then consider a relative error to be $\frac{E_{\text{meas}} - E_{\text{exact}}}{E_{\text{exact}}} \equiv \epsilon < 0.01$ (where E_{meas} is the value of the quantity analyzed with fixed truncation and E_{exact} is the reference value). In the interval of interest, $1.4 \leq \beta \leq 10^2$, we select which, between electric basis ($l = 7$) and magnetic basis ($l = 7$ and J), gives us the lowest relative error. The results are then used to determine where to switch between both bases in the step scaling procedure, as described in the Section “Step scaling approach”. We also tested that even with a smaller truncation $l = 3$, and higher discretization, we can reproduce the same results, thus with a lower number of resources, high precision can be still guaranteed. Note that the magnetic basis may have the advantage of needing a lower truncation when $\beta \gg 1$, but in general has a more complicated Hamiltonian.

In the following, we will show the data of the static forces $F(r_1 = 1, g)$ and $F(r_2 = \sqrt{5}, g)$ with $l = 3$, the other case follows a similar procedure. The selection method systematically explores the potential values of



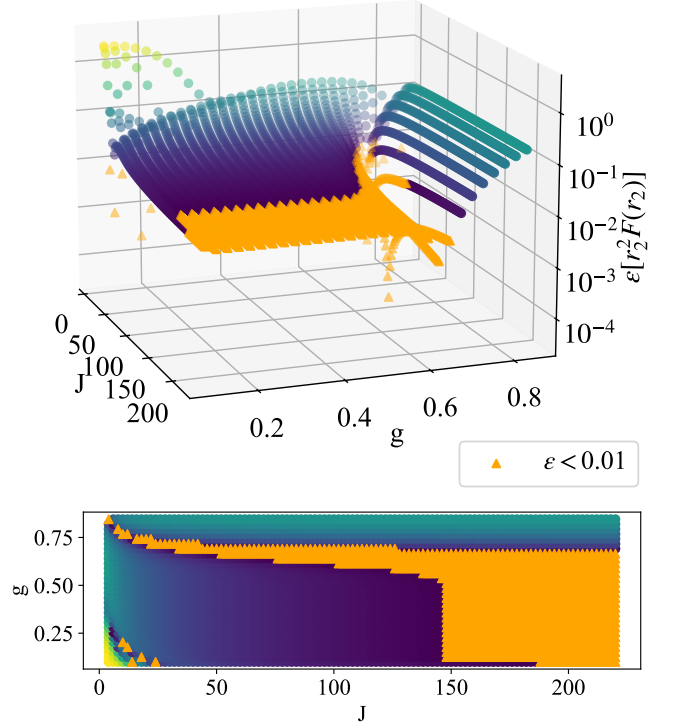
Supplementary Fig. 8: **Relative error for static force, in the magnetic basis.** (top) Relative error for static force $r_1^2 F(r_1 = 1, g)$ in the magnetic basis at $l = 3$. The *triangles* correspond to an error below the threshold, $\epsilon < 0.01$. (bottom) 2D projection heatmap on the (J, g) plane. For small g , a larger discretization J is required to reach an accurate result. When increasing g , the J parameter must be decreased to capture more states.

J with a fixed l for the magnetic basis. In the top panel of Supplementary Fig. 8, we present the relative error ϵ for the quantity $r_1^2 F(r_1 = 1, g)$ across various ranges of g and J (horizontal axes). The results that satisfy the condition $\epsilon < 0.01$ are considered suitable for the scaling approach and are highlighted with *triangles*. Examining the bottom panel, which displays the same data with a color-map, we observe that for small couplings, a discretization of at least $J > 130$ is required. Conversely, in the stronger coupling region, the magnetic data demonstrate higher precision only for specific values of J . This behavior is in line with expectations, as an increase in g should allow for the inclusion of more states within the truncation, ultimately favouring $J = l + 1$. However, the fluctuations are remarkably pronounced and the optimal value of J strongly depends on the considered value of g . Given the wide range of couplings scanned during the step scaling process, adjusting the discretization for mi-



Supplementary Fig. 9: **Comparison between electric and magnetic basis results for the renormalized coupling.** $r_1^2 F(r_1 = 1, g)$: the *small dots* correspond to results with $l_{el} = 7$ in the electric basis and with relative errors ϵ lower than the corresponding ones in the magnetic basis. At $g \sim 0.383$ and below, the electric data have $\epsilon \geq 0.01$ (*crosses*). At this point, the magnetic basis ($l_{mag} = 3$) is considered for the computation. For this regime, a discretization parameter J within the *triangles* region is selected.

nor intervals of g is deemed inefficient. Consequently, we opt for the magnetic basis only with a stable configuration of input parameters. The comparison procedure, depicted in Supplementary Fig. 9, is outlined through the following steps: initially, we identify the data in the electric basis ($l_{el} = 7$) that yields a relative error at a specific g , lower compared to the magnetic basis. Subsequently, we sequentially scan from top to bottom until we determine the minimum bare coupling at which the electric basis remains viable. This condition is established when the results exhibit a relative error below the fixed threshold of $\epsilon(\text{el. basis}) < 0.01$. At this critical coupling ($g \sim 0.383$), we switch to the magnetic formulation ($l_{mag} = 3$) and select a discretization parameter J that satisfies the above condition. Since the dimension of the Hilbert space remains independent of the choice of J we opt for a large discretization value that can accommodate both $r_1^2 F(r_1, g)$ and $r_2^2 F(r_2, g)$ calculations. An equivalent analysis can be repeated for the second static force and compute $r_2^2 F(r_2 = \sqrt{5}, g)$, see Supplementary Fig. 10 for magnetic basis convergence and Supplementary Fig. 11 for electric/magnetic comparison. This analysis was used for the two sets of distances in the Sections “Step scaling results for static forces $F(r_1 = 1, g)$ and $F(r_2 = \sqrt{5}, g)$ ” and “Step scaling results for static forces $F(r_1 = \sqrt{2}, g)$ and $F(r_2 = \sqrt{5}, g)$ ”.



Supplementary Fig. 10: **Relative error for the static force computed in the magnetic basis.** (*top*)

Relative error for $r_2^2 F(r_2 = \sqrt{5}, g)$ at ($l = 3$): the *triangles* correspond to an error below the threshold, $\epsilon < 0.01$. (*bottom*) 2D projection on the plane (J, g).

For small g , a larger discretization J is required to reach an accurate result. When increasing g , the J parameter must be decreased to capture more states.

IV. SUPPLEMENTARY NOTE 4: MATTER FIELDS

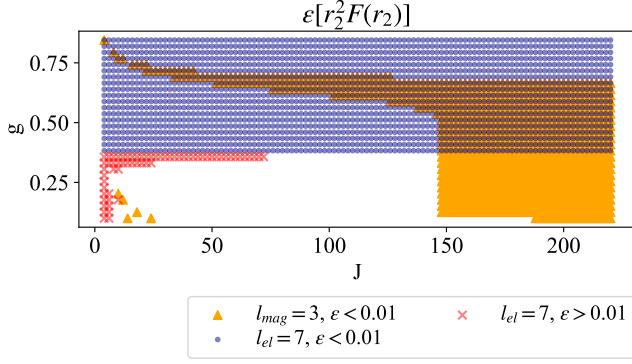
In this appendix, we aim to explain the fermionic part of the QED Hamiltonian for completeness. The starting point is the definition of the Dirac matrices in a $(2+1)$ -dimensional theory. In the following, we will consider the metric $g^{\mu\nu} = (+, -)$. We have γ^0 hermitian and γ^i anti-hermitian satisfying,

$$(\gamma^0)^2 = \mathbb{1}, \quad (\gamma^i)^2 = -\mathbb{1}. \quad (6)$$

In this work, we have chosen the γ -matrices as,

$$\gamma_0 = \sigma_z, \quad \gamma_1 = -i\sigma_y, \quad \gamma_2 = -i\sigma_x, \quad (7)$$

where σ_i , $i = x, y, z$ are Pauli matrices. The fermionic Hamiltonian on a lattice of size N_x (N_y) in x (y) direction is written as,



Supplementary Fig. 11: **Comparison between electric and magnetic basis results for the renormalized coupling.** $r_2^2 F(r_2 = \sqrt{5}, g)$: the *small dots* correspond to results with $l_{el} = 7$ in the electric basis and with relative errors ϵ lower than the corresponding ones in the magnetic basis. At $g \sim 0.383$ and below, the electric data have $\epsilon \geq 0.01$ (*crosses*). At this point, the magnetic basis ($l_{mag} = 3$) is considered for the computation. For this regime, a discretization parameter J within the *triangles* region is selected.

$$H = -i \sum_{\mathbf{r}=(0,0)}^{(N_x, N_y)} \left[\bar{\psi}(\mathbf{r}) \gamma^1 \frac{U_{\mathbf{r},x} \psi(r_x + 1, r_y) - U_{\mathbf{r},-x}^\dagger \psi(r_x - 1, r_y)}{2a} + \bar{\psi}(\mathbf{r}) \gamma^2 \frac{U_{\mathbf{r},y} \psi(r_x, r_y + 1) - U_{\mathbf{r},-y}^\dagger \psi(r_x, r_y - 1)}{2a} + m \bar{\psi}(\mathbf{r}) \psi(\mathbf{r}) \right], \quad (8)$$

where the first two terms represent the two covariant derivatives in x and y direction and belong to the kinetic part, the last line defines the mass and $\mathbf{r} = (r_x, r_y)$ represents the lattice site. Here and in the rest of this section, we omit, for simplicity, the operator notation $\hat{O} \rightarrow O$. With a two-components spinor $\psi = (\psi_1, \psi_2)^t$ and a staggered formulation [15], Eq. (8) can be recast and the fermionic fields are selected to have a single component for each site, with arbitrary choice ψ_1 (ψ_2) on even (odd) sites or vice-versa. As a last step, ψ_1 and ψ_2 can be replaced with a single component field ϕ , obtaining Eq. (7) and Eq. (8) in the main text.

We will now discuss a few properties of this formulation. Starting from the Dirac equation $(i\hat{D} - m)\psi = 0$, we have

$$i\gamma^0 \partial_0 \psi + i\gamma^1 \partial_1 \psi + i\gamma^2 \partial_2 \psi = m\psi, \quad (9)$$

or in the Schrödinger form,

$$i \frac{\partial \psi}{\partial t} = H\psi, \quad H = \gamma^0 \gamma^1 p_1 + \gamma^0 \gamma^2 p_2 + \gamma^0 m, \quad (10)$$

where $p_j \rightarrow -i\partial_j$. Explicitly substituting the γ -matrices from Eq. (7), one gets,

$$i\dot{\psi} = -i \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} \partial_x \psi - i \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \partial_y \psi + m \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \psi, \quad (11)$$

and in terms of the two components,

$$i \begin{pmatrix} \dot{\psi}_1(\mathbf{r}) \\ \dot{\psi}_2(\mathbf{r}) \end{pmatrix} = i\partial_x \begin{pmatrix} \psi_2(\mathbf{r}) \\ \psi_1(\mathbf{r}) \end{pmatrix} + \partial_y \begin{pmatrix} -\psi_2(\mathbf{r}) \\ \psi_1(\mathbf{r}) \end{pmatrix} + m \begin{pmatrix} \psi_1(\mathbf{r}) \\ -\psi_2(\mathbf{r}) \end{pmatrix}. \quad (12)$$

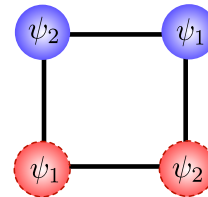
Following Refs. [15, 16], we select only the kinetic part of Eq. (12) and rewrite it as

$$\begin{pmatrix} \dot{\psi}_1(\mathbf{r}) \\ \dot{\psi}_2(\mathbf{r}) \end{pmatrix} = \partial_x \begin{pmatrix} \psi_2(\mathbf{r}) \\ \psi_1(\mathbf{r}) \end{pmatrix} + \partial_y \begin{pmatrix} i\psi_2(\mathbf{r}) \\ -i\psi_1(\mathbf{r}) \end{pmatrix}, \quad (13)$$

or in compact form,

$$\dot{\psi} = \sigma_x \partial_x \psi - \sigma_y \partial_y \psi. \quad (14)$$

We consider the upper components of Eq. (13) and place ψ_1 on a site. Then shifting one site in the $\pm x$ direction couples ψ_1 to ψ_2 . Similarly, a shift of one site in the $\pm y$ direction results in a coupling between ψ_1 to ψ_2 . Therefore, to yield a coherent geometric interpretation of Eq. (13), the components should be arranged as illustrated in Supplementary Fig. 12.



Supplementary Fig. 12: **Geometric interpretation of Dirac equation for a two-component spinor on a planar lattice.** In 2D, each component appears twice on the unit square, once on a $y = \text{const.}$ plane (*lower sites*) and again on a $y = \text{const.} + a$ plane (*upper sites*).

Note that each component resides twice within the unit square: once on a $y = \text{const.}$ plane and again on the subsequent $y = \text{const.} + a$ plane. Consequently, in the continuum limit, two fermion fields will emerge within this framework. To distinguish between them, we label the fields on the lower $y = \text{const.}$ plane in Supplementary Fig. 12 as f_i , $i = 1, 2$, and those on the upper $y = \text{const.} +$

a plane as g_i , $i = 1, 2$. In this terminology, the Dirac equation, Eq. (13), transforms into:

$$\begin{cases} \dot{f} = \sigma_x \partial_x f - \sigma_y \partial_y g \\ \dot{g} = \sigma_x \partial_x g - \sigma_y \partial_y f. \end{cases} \quad (15a)$$

$$(15b)$$

Now we distinguish two distinct species: the equation of motion for the sum $u = f + g$ satisfies

$$\dot{u} = (\sigma_x \partial_x - \sigma_y \partial_y)u, \quad (16)$$

and produces one fermion in the continuum limit. The difference $\tilde{d} = f - g$ satisfies

$$\dot{\tilde{d}} = (\sigma_x \partial_x + \sigma_y \partial_y)\tilde{d}, \quad (17)$$

which is not a Dirac equation because of the different sign in the last term. However, this can be changed via a unitary transformation, $d = \sigma_x \tilde{d}$, which gives

$$\dot{d} = (\sigma_x \partial_x - \sigma_y \partial_y)d. \quad (18)$$

In summary, this fermion method generates two massless fermion fields in the continuum limit. We are, therefore,

free to interpret u and d as the members of an isodoublet, $(u, d)^t$.

Another interesting property of a formulation with two-component spinors involves the mass term of the Hamiltonian. In Ref. [17] it is described how considering spinors with two components yields parity breaking in the mass term, where a parity transformation is defined as,

$$\begin{pmatrix} \psi_1(x, y) \\ \psi_2(x, y) \end{pmatrix} \xrightarrow{P} \begin{pmatrix} \psi_2(-x, y) \\ \psi_1(-x, y) \end{pmatrix}, \quad (19)$$

and it also acts on the vector fields,

$$\begin{pmatrix} A_1(x, y) \\ A_2(x, y) \end{pmatrix} \xrightarrow{P} \begin{pmatrix} -A_1(-x, y) \\ A_2(-x, y) \end{pmatrix}, \quad (20)$$

i.e. the U operators will be

$$U_{\mathbf{r}, \mathbf{r}+e_x}(x, y) \xrightarrow{P} U_{\mathbf{r}, \mathbf{r}+e_x}^\dagger(-x, y) \quad (21a)$$

$$U_{\mathbf{r}, \mathbf{r}+e_y}(x, y) \xrightarrow{P} U_{\mathbf{r}, \mathbf{r}+e_y}(-x, y). \quad (21b)$$

As also described in Ref. [17], for a parity-conserving theory, one should then consider a study of four-component spinors. Since this is beyond the purpose of this work, we will not further discuss it.

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