

Hamiltonian Formulation of Gauge Theories and its Use for Quantum Simulation

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Outline

Lecture 1a: What are Photons?

Lecture 1b: Kogut-Susskind Hamiltonian for $U(1)$ Gauge Theory

Lecture 2a: $U(1)$ Quantum Link Models

Lecture 2b: The Sign Problem and Quantum Simulation

Lecture 3a: Kogut-Susskind Hamiltonian for $SU(N)$ Gauge Theory

Lecture 3b: Non-Abelian Quantum Link Models

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Different descriptions of dynamical Abelian gauge fields:

Maxwell's classical electromagnetic gauge fields

$$\vec{\nabla} \cdot \vec{E}(\vec{x}, t) = \rho(\vec{x}, t), \quad \vec{\nabla} \cdot \vec{B}(\vec{x}, t) = 0, \quad \vec{B}(\vec{x}, t) = \vec{\nabla} \times \vec{A}(\vec{x}, t)$$

Quantum Electrodynamics (QED) for perturbative treatment

$$E_i = -i \frac{\partial}{\partial A_i}, \quad [E_i(\vec{x}), A_j(\vec{x}')] = i \delta_{ij} \delta(\vec{x} - \vec{x}'), \quad [\vec{\nabla} \cdot \vec{E} - \rho] |\Psi[A]\rangle = 0$$

Wilson's $U(1)$ lattice gauge theory for classical simulation

$$U_{xy} = \exp \left(ie \int_x^y d\vec{l} \cdot \vec{A} \right) = \exp(i\varphi_{xy}) \in U(1), \quad E_{xy} = -i \frac{\partial}{\partial \varphi_{xy}}$$

$$[E_{xy}, U_{xy}] = U_{xy}, \quad \left[\sum_i (E_{x, x+\hat{i}} - E_{x-\hat{i}, x}) - \rho \right] |\Psi[U]\rangle = 0$$

$U(1)$ quantum link models for quantum simulation

$$U_{xy} = S_{xy}^+, \quad U_{xy}^\dagger = S_{xy}^-, \quad E_{xy} = S_{xy}^3,$$

$$[E_{xy}, U_{xy}] = U_{xy}, \quad [E_{xy}, U_{xy}^\dagger] = -U_{xy}^\dagger, \quad [U_{xy}, U_{xy}^\dagger] = 2E_{xy}$$

Canonical Quantization of the Electromagnetic Field

The homogeneous Maxwell equations

$$\vec{\nabla} \times \vec{E}(\vec{x}, t) + \frac{1}{c} \partial_t \vec{B}(\vec{x}, t) = 0, \quad \vec{\nabla} \cdot \vec{B}(\vec{x}) = 0$$

are satisfied when we introduce scalar and vector potentials

$$\vec{E}(\vec{x}, t) = -\vec{\nabla} \phi(\vec{x}, t) - \frac{1}{c} \partial_t \vec{A}(\vec{x}, t), \quad \vec{B}(\vec{x}, t) = \vec{\nabla} \times \vec{A}(\vec{x}, t)$$

Under a gauge transformation

$$\phi'(\vec{x}, t) = \phi(\vec{x}, t) - \frac{1}{c} \partial_t \alpha(\vec{x}, t), \quad \vec{A}'(\vec{x}, t) = \vec{A}(\vec{x}, t) - \vec{\nabla} \alpha(\vec{x}, t)$$

the electromagnetic fields are invariant

$$\begin{aligned} \vec{E}'(\vec{x}, t) &= -\vec{\nabla} \phi'(\vec{x}, t) - \frac{1}{c} \partial_t \vec{A}'(\vec{x}, t) = -\vec{\nabla} \phi'(\vec{x}, t) - \frac{1}{c} \vec{\nabla} \partial_t \alpha(\vec{x}, t) \\ &\quad - \frac{1}{c} \partial_t \vec{A}(\vec{x}, t) + \frac{1}{c} \partial_t \vec{\nabla} \alpha(\vec{x}, t) = \vec{E}(\vec{x}, t) \\ \vec{B}'(\vec{x}, t) &= \vec{\nabla} \times \vec{A}'(\vec{x}, t) = \vec{\nabla} \times \vec{A}(\vec{x}, t) - \vec{\nabla} \times \vec{\nabla} \alpha(\vec{x}, t) = \vec{B}(\vec{x}, t) \end{aligned}$$

Relativistic Formulation of Electrodynamics with 4-Vectors

$$x^0 = ct, \quad x^\mu = (x^0, \vec{x}), \quad \partial_\mu = \left(\frac{1}{c} \partial_t, \vec{\nabla} \right), \quad A^\mu(x) = (\phi(\vec{x}, t), \vec{A}(\vec{x}, t))$$

The field strength tensor

$$\begin{aligned} F^{\mu\nu}(x) &= \partial^\mu A^\nu(x) - \partial^\nu A^\mu(x) \\ &= \begin{pmatrix} 0 & -E_x(\vec{x}, t) & -E_y(\vec{x}, t) & -E_z(\vec{x}, t) \\ E_x(\vec{x}, t) & 0 & -B_z(\vec{x}, t) & B_y(\vec{x}, t) \\ E_y(\vec{x}, t) & B_z(\vec{x}, t) & 0 & -B_x(\vec{x}, t) \\ E_z(\vec{x}, t) & -B_y(\vec{x}, t) & B_x(\vec{x}, t) & 0 \end{pmatrix} \end{aligned}$$

is invariant under gauge transformations

$$\begin{aligned} A'^\mu(x) &= A^\mu(x) - \partial^\mu \alpha(x), \\ F'^{\mu\nu}(x) &= \partial^\mu A'^\nu(x) - \partial^\nu A'^\mu(x) \\ &= \partial^\mu A^\nu(x) - \partial^\nu A^\mu(x) - \partial^\mu \partial^\nu \alpha(x) + \partial^\nu \partial^\mu \alpha(x) = F^{\mu\nu}(x) \end{aligned}$$

From the Lagrangian to the Hamilton Density

$$\mathcal{L}(\partial^\mu A^\nu) = -\frac{1}{4}F_{\mu\nu}(x)F^{\mu\nu}(x) = \frac{1}{2} \left(\vec{E}(x)^2 - \vec{B}(x)^2 \right)$$

Temporal gauge fixing

$$A^0(x) = \phi(\vec{x}, t) = 0$$

Canonically conjugate momenta

$$E_i(x) = -\partial^0 A^i(x) \ , \ \Pi_i(x) = \frac{\delta \mathcal{L}}{\delta \partial^0 A^i(x)} = \partial^0 A^i(x) = -E_i(x)$$

Classical Hamilton density

$$\begin{aligned} \mathcal{H}(A^i, \Pi_i) &= \Pi_i(x) \partial^0 A^i(x) - \mathcal{L} = \frac{1}{2} (\Pi_i(x) \Pi_i(x) + B_i(x) B_i(x)) \\ &= \frac{1}{2} (E_i(x) E_i(x) + B_i(x) B_i(x)) \end{aligned}$$

Classical Hamilton function

$$H = \int d^3x \ \mathcal{H} = \int d^3x \ \frac{1}{2} \left[\Pi_i(\vec{x}) \Pi_i(\vec{x}) + \epsilon_{ijk} \partial_j A^k(\vec{x}) \epsilon_{ilm} \partial_l A^m(\vec{x}) \right]$$

From classical to quantum electrodynamics

Canonical commutation relations

$$[\hat{A}^i(\vec{x}), \hat{\Pi}_j(\vec{y})] = i \delta_{ij} \delta(\vec{x} - \vec{y}) , \quad [\hat{A}^i(\vec{x}), \hat{A}^j(\vec{y})] = [\hat{\Pi}_i(\vec{x}), \hat{\Pi}_j(\vec{y})] = 0$$

Conjugate momentum operator

$$\hat{\Pi}_i(\vec{x}) = -i \frac{\delta}{\delta A^i(\vec{x})}$$

Hamilton operator of the electromagnetic field

$$\hat{H} = \int d^3x \frac{1}{2} \left[\hat{\Pi}_i(\vec{x}) \hat{\Pi}_i(\vec{x}) + \epsilon_{ijk} \partial_j \hat{A}^k(\vec{x}) \epsilon_{ilm} \partial_l \hat{A}^m(\vec{x}) \right]$$

Fourier transform

$$\hat{A}^i(\vec{p}) = \int d^3x \hat{A}^i(\vec{x}) \exp(-i \vec{p} \cdot \vec{x}) , \quad \hat{A}^i(\vec{p})^\dagger = \hat{A}^i(-\vec{p})$$

$$\hat{\Pi}_i(\vec{p}) = \int d^3x \hat{\Pi}_i(\vec{x}) \exp(-i \vec{p} \cdot \vec{x}) , \quad \hat{\Pi}_i(\vec{p})^\dagger = \hat{\Pi}_i(-\vec{p})$$

$$[\hat{A}^i(\vec{p}), \hat{\Pi}_i(\vec{q})] = i (2\pi)^3 \delta_{ij} \delta(\vec{p} + \vec{q})$$

$$[\hat{A}^i(\vec{p}), \hat{A}^j(\vec{q})] = [\hat{\Pi}_i(\vec{p}), \hat{\Pi}_j(\vec{q})] = 0$$

Diagonalization of the Hamiltonian

$$\hat{H} = \frac{1}{(2\pi)^3} \int d^3p \frac{1}{2} \left[\hat{\Pi}_i(\vec{p})^\dagger \hat{\Pi}_i(\vec{p}) + \epsilon_{ijk} p_j \hat{A}^k(\vec{p})^\dagger \epsilon_{ilm} p_l \hat{A}^m(\vec{p}) \right]$$

Gauss law

$$\vec{\nabla} \cdot \hat{\vec{E}}(\vec{x}) |\Psi\rangle = 0 \Rightarrow p_i \hat{\Pi}_i(\vec{p}) |\Psi\rangle = 0$$

Quadratic form of the magnetic field term

$$\epsilon_{ijk} p_j \hat{A}^k(\vec{p})^\dagger \epsilon_{ilm} p_l \hat{A}^m(\vec{p}) =$$
$$(\hat{A}^1(\vec{p})^\dagger, \hat{A}^2(\vec{p})^\dagger, \hat{A}^3(\vec{p})^\dagger) \begin{pmatrix} \vec{p}^2 - p_1^2 & -p_1 p_2 & -p_1 p_3 \\ -p_2 p_1 & \vec{p}^2 - p_2^2 & -p_2 p_3 \\ -p_3 p_1 & -p_3 p_2 & \vec{p}^2 - p_3^2 \end{pmatrix} \begin{pmatrix} \hat{A}^1(\vec{p}) \\ \hat{A}^2(\vec{p}) \\ \hat{A}^3(\vec{p}) \end{pmatrix}$$

Symmetric matrix

$$\mathcal{M}(\vec{p})_{ij} = \vec{p}^2 (\delta_{ij} - e_{pi} e_{pj}) \quad , \quad \vec{e}_p = \vec{p}/|\vec{p}|$$

$$\vec{e}_1 \cdot \vec{e}_p = \vec{e}_2 \cdot \vec{e}_p = 0 \quad , \quad \vec{e}_1 \cdot \vec{e}_2 = 0 \quad , \quad \vec{e}_1 \times \vec{e}_2 = \vec{e}_p \quad , \quad \vec{e}_\pm = \frac{1}{\sqrt{2}} (\vec{e}_1 \pm i \vec{e}_2)$$

$$\vec{e}_\pm^* \cdot \vec{e}_\pm = 1 \quad , \quad \vec{e}_\pm \cdot \vec{e}_p = 0 \quad , \quad \vec{e}_-^* \cdot \vec{e}_+ = 0 \quad , \quad \vec{e}_- \times \vec{e}_+ = i \vec{e}_p \quad (1)$$

Unitary transformation diagonalizes $\mathcal{M}(\vec{p})$

$$U(\vec{p}) = \begin{pmatrix} e_{+1} & e_{+2} & e_{+3} \\ e_{p1} & e_{p2} & e_{p3} \\ e_{-1} & e_{-2} & e_{-3} \end{pmatrix}, \quad U(\vec{p})\mathcal{M}(\vec{p})U(\vec{p})^\dagger = \vec{p}^2 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$
$$\begin{pmatrix} \hat{A}_+(\vec{p}) \\ \hat{A}_p(\vec{p}) \\ \hat{A}_-(\vec{p}) \end{pmatrix} = U(\vec{p}) \begin{pmatrix} \hat{A}^1(\vec{p}) \\ \hat{A}^2(\vec{p}) \\ \hat{A}^3(\vec{p}) \end{pmatrix}, \quad \begin{pmatrix} \hat{\Pi}_+(\vec{p}) \\ \hat{\Pi}_p(\vec{p}) \\ \hat{\Pi}_-(\vec{p}) \end{pmatrix} = U(\vec{p}) \begin{pmatrix} \hat{\Pi}_1(\vec{p}) \\ \hat{\Pi}_2(\vec{p}) \\ \hat{\Pi}_3(\vec{p}) \end{pmatrix}$$

Diagonalized Hamilton operator

$$\begin{aligned} \hat{H} = & \frac{1}{(2\pi)^3} \int d^3p \frac{1}{2} \left[\hat{\Pi}_+(\vec{p})^\dagger \hat{\Pi}_+(\vec{p}) + \vec{p}^2 \hat{A}_+(\vec{p})^\dagger \hat{A}_+(\vec{p}) \right. \\ & \left. + \hat{\Pi}_-(\vec{p})^\dagger \hat{\Pi}_-(\vec{p}) + \vec{p}^2 \hat{A}_-(\vec{p})^\dagger \hat{A}_-(\vec{p}) + \hat{\Pi}_p(\vec{p})^\dagger \hat{\Pi}_p(\vec{p}) \right] \end{aligned}$$

Hamilton operator commutes with Gauss law constraint

$$[\hat{H}, \hat{\Pi}_p(\vec{p})] = 0, \quad \hat{\Pi}_p(\vec{p}) = U(\vec{p})_{pi} \hat{\Pi}_i(\vec{p}) = -e_{pi} \hat{E}_i(\vec{p}) = -\frac{\vec{p}}{|\vec{p}|} \cdot \hat{\vec{E}}(\vec{p})$$

Creation and annihilation operators for photons

$$\begin{aligned}\hat{a}_{\pm}(\vec{p}) &= \frac{1}{\sqrt{2}} \left[\sqrt{|\vec{p}|} \hat{A}_{\pm}(\vec{p}) + \frac{i}{\sqrt{|\vec{p}|}} \hat{P}_{\pm}(\vec{p}) \right] \\ \hat{a}_{\pm}(\vec{p})^{\dagger} &= \frac{1}{\sqrt{2}} \left[\sqrt{|\vec{p}|} \hat{A}_{\pm}(\vec{p})^{\dagger} - \frac{i}{\sqrt{|\vec{p}|}} \hat{P}_{\pm}(\vec{p})^{\dagger} \right]\end{aligned}$$

Commutation relations

$$\begin{aligned}[\hat{a}_{\pm}(\vec{p}), \hat{a}_{\pm}(\vec{q})^{\dagger}] &= (2\pi)^3 \delta(\vec{p} - \vec{q}) \\ [\hat{a}_{+}(\vec{p}), \hat{a}_{-}(\vec{q})^{\dagger}] &= [\hat{a}_{-}(\vec{p}), \hat{a}_{+}(\vec{q})^{\dagger}] = 0 \\ [\hat{a}_{\pm}(\vec{p}), \hat{a}_{\pm}(\vec{q})] &= [\hat{a}_{\pm}(\vec{p})^{\dagger}, \hat{a}_{\pm}(\vec{q})^{\dagger}] = 0\end{aligned}\quad (2)$$

Hamilton operator in the physical sector

$$\hat{H} = \frac{1}{(2\pi)^3} \int d^3p \, |\vec{p}| \left(\hat{a}_{+}(\vec{p})^{\dagger} \hat{a}_{+}(\vec{p}) + \hat{a}_{-}(\vec{p})^{\dagger} \hat{a}_{-}(\vec{p}) + V \right) \quad (3)$$

Vacuum and photon states

$$\hat{a}_{\pm}(\vec{p})|0\rangle = 0, \quad \hat{H}|0\rangle = E_0|0\rangle$$

$$|\vec{p}, \pm\rangle = \hat{a}_{\pm}(\vec{p})^{\dagger}|0\rangle, \quad \hat{H}|\vec{p}, \pm\rangle = E(\vec{p})|\vec{p}, \pm\rangle, \quad E(\vec{p}) - E_0 = |\vec{p}|$$

Momentum operator and momentum of photons

$$\begin{aligned}\hat{\vec{P}} &= \int d^3x \frac{1}{2} \left(\hat{\vec{E}}(\vec{x}) \times \hat{\vec{B}}(\vec{x}) - \hat{\vec{B}}(\vec{x}) \times \hat{\vec{E}}(\vec{x}) \right) \\ &= \frac{1}{(2\pi)^3} \int d^3p \vec{p} \left(\hat{a}_{+}(\vec{p})^{\dagger} \hat{a}_{+}(\vec{p}) + \hat{a}_{-}(\vec{p})^{\dagger} \hat{a}_{-}(\vec{p}) \right) \\ \left[\hat{\vec{P}}, \hat{a}_{\pm}(\vec{p})^{\dagger} \right] &= \vec{p} \hat{a}_{\pm}(\vec{p})^{\dagger} \Rightarrow \hat{\vec{P}}|\vec{p}, \pm\rangle = \vec{p} |\vec{p}, \pm\rangle\end{aligned}\quad (4)$$

Angular momentum operator and helicity of photons

$$\begin{aligned}\hat{\vec{J}} &= \int d^3x \vec{x} \times \frac{1}{2} \left(\hat{\vec{E}}(\vec{x}) \times \hat{\vec{B}}(\vec{x}) - \hat{\vec{B}}(\vec{x}) \times \hat{\vec{E}}(\vec{x}) \right) \\ [\hat{P}_i, \hat{J}_j] &= i\epsilon_{ijk} \hat{P}_k \Rightarrow [\hat{\vec{P}}, \hat{\vec{P}} \cdot \hat{\vec{J}}] = 0 \\ \left[\hat{\vec{J}} \cdot \vec{e}_p, \hat{a}_{\pm}(\vec{p})^{\dagger} \right] &= \pm \hat{a}_{\pm}(\vec{p})^{\dagger} \Rightarrow \hat{\vec{J}} \cdot \vec{e}_p |\vec{p}, \pm\rangle = \pm |\vec{p}, \pm\rangle\end{aligned}\quad (5)$$

Homework: Recapitulate Lecture 1a and verify eqs.(1-5)

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Wilson's concept of a parallel transporter

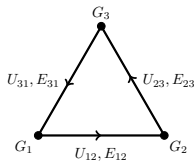
$$U_{xy} = \exp \left[ie \int_{x_k}^{x_k+a} dx_k A_k(x) \right] \in U(1)$$

Behavior under gauge transformations

$$\begin{aligned} A_k(x)' &= A_k(x) - \partial_k \alpha(x) \Rightarrow \\ U'_{xy} &= \exp \left[ie \int_{x_k}^{x_k+a} dx_k A'_k(x) \right] \\ &= \exp \left[ie \int_{x_k}^{x_k+a} dx_k \{ A_k(x) - \partial_k \alpha(x) \} \right] \\ &= \exp \left[ie \left\{ \int_{x_k}^{x_k+a} dx_k A_k(x) + \alpha(x) - \alpha(y) \right\} \right] \\ &= \Omega_x U_{xy} \Omega_y^\dagger, \quad \Omega_x = \exp [i\alpha(x)] \in U(1) \end{aligned}$$

Quantum mechanical analog “particle” on a circle $S^1 = U(1)$

$$\begin{aligned} U &= \exp(i\varphi), \quad U^\dagger = \exp(-i\varphi), \quad E = -i\partial_\varphi \\ [E, U] &= U, \quad [E, U^\dagger] = -U^\dagger, \quad [U, U^\dagger] = 0 \end{aligned}$$



Three analog “particles” on a plaquette

$$E_{12} = -i\partial_{\varphi_{12}} , \quad E_{23} = -i\partial_{\varphi_{23}} , \quad E_{31} = -i\partial_{\varphi_{31}}$$

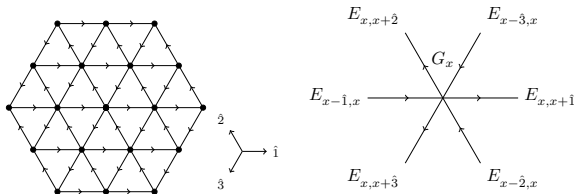
Three-“particle” Hamiltonian

$$\begin{aligned} H &= T_{12} + T_{23} + T_{31} + V_{123} \\ &= \frac{E_{12}^2}{2I} + \frac{E_{23}^2}{2I} + \frac{E_{31}^2}{2I} - \frac{1}{e^2} \cos(\varphi_1 + \varphi_2 + \varphi_3) \\ &= \frac{E_{12}^2}{2I} + \frac{E_{23}^2}{2I} + \frac{E_{31}^2}{2I} - \frac{1}{2e^2} (U_{12} U_{23} U_{31} + U_{31}^\dagger U_{23}^\dagger U_{12}^\dagger) \end{aligned}$$

Invariance against relative rotations

$$\begin{aligned} G_1 &= E_{12} - E_{31} , \quad G_2 = E_{23} - E_{12} , \quad G_3 = E_{31} - E_{23} \\ [H, G_1] &= [H, G_2] = [H, G_3] = 0 \end{aligned} \tag{6}$$

Many “particles” in S^1 forming a $U(1)$ lattice gauge theory



$$H = \frac{e^2}{2} \sum_{\langle xy \rangle} E_{xy}^2 - \frac{1}{2e^2} \sum_{\langle xyz \rangle} (U_{xy} U_{yz} U_{zx} + U_{zx}^\dagger U_{yz}^\dagger U_{xy}^\dagger) , \quad I = \frac{1}{e^2}$$

Link-based operator algebra

$$\begin{aligned} [E_I, E_{I'}] &= 0 , & [E_I, U_{I'}] &= i\delta_{II'} U_I , & [E_I, U_{I'}^\dagger] &= -i\delta_{II'} U_I^\dagger \\ [U_I, U_{I'}] &= [U_I^\dagger, U_{I'}^\dagger] = [U_I, U_{I'}^\dagger] &= 0 \end{aligned}$$

Invariance against gauge transformations

$$G_x = \sum_k (E_{x,x+\hat{k}} - E_{x-\hat{k},x}) , \quad [G_x, G_y] = 0 , \quad [H, G_x] = 0 \quad (7)$$

General gauge transformations and Gauss law

$$V = \prod_x \exp(i\alpha_x G_x) , \quad V U_{xy} V^\dagger = \Omega_x U_{xy} \Omega_y^\dagger \quad (8)$$

States with external charges $Q_x \in \mathbb{Z}$

$$G_x |\Psi, Q\rangle = Q_x |\Psi, Q\rangle , \quad Q = \{Q_x\}$$

Standard Gauss law

$$G_x |\Psi\rangle = 0$$

Canonical quantum statistical partition function

$$Z_Q = \text{Tr}[\exp(-\beta H) P_Q]$$

Potential between external charges $Q_x = 1, Q_y = -1$

$$\frac{Z_Q}{Z} = \exp(-\beta V(x-y)) , \quad V(x-y) \sim \sigma |x-y|$$

Homework: Recapitulate Lecture 1b and verify eqs.(6-8).

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