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Quantum optimization via four-body Rydberg gates

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A large ongoing research effort focuses on obtaining a quantum advantage in the solution of combinatorial optimization problems on near-term quantum devices. A particularly promising platform implementing quantum optimization algorithms are arrays of trapped neutral atoms, laser-coupled to highly excited Rydberg states. However, encoding combinatorial optimization problems in atomic arrays is challenging due to limited inter-qubit connectivity of the native finite-range interactions. Here we present a four-body Rydberg parity gate, enabling a direct and straightforward implementation of the parity architecture, a scalable architecture for encoding arbitrarily connected interaction graphs. Our gate relies on adiabatic laser pulses and is fully programmable by adjusting two hold-times during operation. We numerically demonstrate implementations of the quantum approximate optimization algorithm (QAOA) for small-scale test problems. Variational optimization steps can be implemented with a constant number of system manipulations, paving the way for experimental investigations of QAOA beyond the reach of numerical simulations.

Introduction—Currently available quantum devices are capable of generating controlled dynamics challenging numerical simulations on even the most powerful classical supercomputers [1–3]. These quantum devices will have up to a few hundred qubits available, without error correction, and have been termed Noisy Intermediate Scale Quantum (NISQ) devices. A key challenge for the field of quantum technology at this very moment is to find ways of putting the computational power of near-term quantum devices to good use [4, 5]. In this era of NISQ devices, the development of specialized algorithms, targeting specific problems that provide a structural match with the strengths of a particular quantum platform, is thus highly desirable. A strategy of co-design of algorithms and experimental platforms aims at developing scientifically and industrially relevant applications in the near term, before the need for error correction arises.

Here we focus on designing specialized quantum hardware for solving combinatorial optimization problems, using neutral atoms trapped in tweezer arrays, laser-coupled to highly excited Rydberg states [6–15]. The Rydberg states provide strong and tunable interactions, that can be switched on and off by coherently coupling ground and Rydberg states. Combined with single particle operations, the interactions form appealing building blocks for QAOA [16, 17]. There, the goal is to find approximate solutions to combinatorial optimization problems, cast in the form of energy minimization of a general N -spin problem Hamiltonian

$$\hat{H}_P = \sum_i J_i \hat{\sigma}_z^{(i)} + \sum_{i<j} J_{ij} \hat{\sigma}_z^{(i)} \hat{\sigma}_z^{(j)} + \sum_{i<j<k} J_{ijk} \hat{\sigma}_z^{(i)} \hat{\sigma}_z^{(j)} \hat{\sigma}_z^{(k)} + \dots, \quad (1)$$

where $\hat{\sigma}_{\{x,y,z\}}$ denote the Pauli spin operators and

$\{J_i, J_{ij}, J_{ijk}, \dots\}$ are local fields and long-ranged higher-order interactions. QAOA attempts to find low energy solutions, by driving a system of quantum spins alternately with a driver Hamiltonian $\hat{H}_X = \sum_i \hat{\sigma}_x^{(i)}$ and the problem Hamiltonian \hat{H}_P .

Despite the recent universality and quantum advantage results [18–20], various aspects of QAOA’s performance are still under theoretical investigation [21]. On the one hand the existence of barren plateaus [22] and reachability deficits [23–25] suggest strong limitations for QAOA while, on the other hand, parameter concentration effects [26–30] may boost the algorithm’s efficiency. Ultimately, due to QAOA’s heuristic nature, its practical performance in a regime beyond the capability of classical computers is difficult to predict and requires to be experimentally tested.

Recent advances in Rydberg experiments, such as coherent control of atomic states and deterministic atom positioning of hundreds of atoms, make the Rydberg platform a particularly promising target for such investigations. Direct experimental implementations of QAOA with Rydberg atoms are, however, limited by the binary nature of the Rydberg interaction and their polynomially decaying interaction strengths, which only admit scalable experimental implementations of \hat{H}_P for very specific problems [8, 31].

Instead of attempting to directly engineer the spin model version of \hat{H}_P , we adopt the parity architecture [32, 33], a scalable and problem independent quantum hardware blueprint for generic combinatorial optimization problems. Running QAOA then only requires problem dependent single-qubit gates and problem independent multi-qubit phase-gates acting on three or four qubits at the corners of 2×2 plaquettes as (cf. Fig. 1) $U_{\blacksquare}(\gamma) = e^{i\gamma} \Pi_k \hat{\sigma}_z^{(k)}$, where the latter do not naturally

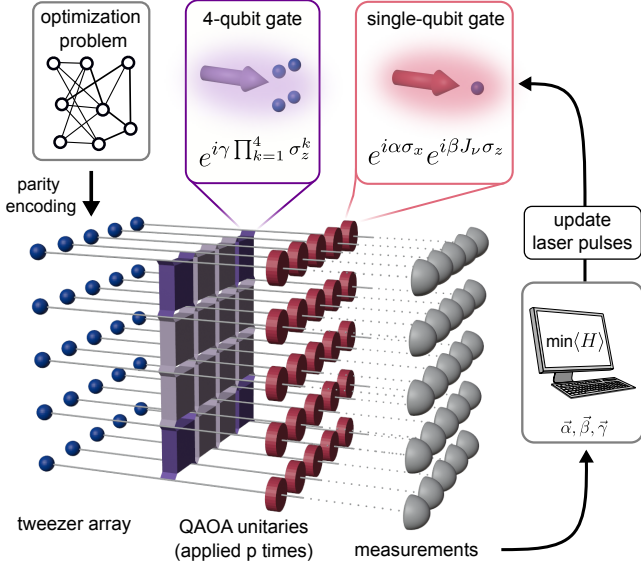


FIG. 1. *Rydberg parity QAOA protocol.* Arbitrarily connected optimization problems can be parity encoded in a regular geometry of neutral atoms trapped in e.g. optical tweezers. After initializing the Rydberg quantum processor in an equal superposition state, generating variational wave functions by applying QAOA unitaries only requires local control of laser fields generating quasi-local four- (square boxes) and single-qubit gates (discs).

exist on the Rydberg platform.

In the following we show how such a gate can be directly engineered between ground state atoms utilizing time-optimal adiabatic laser-coupling to Rydberg states, i.e. without relying on (distinct species) auxiliary qubits [34] or decomposition into two-body gates [35]. We provide a simple two-pulse strategy to program arbitrary phases γ subsequent to a onetime optimization of laser-ramps within parameter-limits given by particular experiments. The entire QAOA can then be implemented on present-day experiments as an optimization of the duration of laser pulses. Below we explain the details and performance of our scheme, and give a numerical demonstration of the QAOA protocol on the Rydberg platform.

Rydberg parity QAOA– The parity hardware architecture provides a blueprint for a problem independent and scalable quantum processor that is tailored to tackle generic combinatorial optimization problems (see Supplemental Material (SM) [36] for a detailed introduction). In short, parity-qubits encode the relative orientation, i.e. the parity, of spins representing the optimization problem, with $J_{ij} \hat{\sigma}_z^{(i)} \hat{\sigma}_z^{(j)} \rightarrow J_\mu \hat{\sigma}_z^{(\mu)}$, $J_{ijk} \hat{\sigma}_z^{(i)} \hat{\sigma}_z^{(j)} \hat{\sigma}_z^{(k)} \rightarrow J_\nu \hat{\sigma}_z^{(\nu)}$ etc., replacing long-range interactions $\{J_{ij}, J_{ijk}, \dots\}$ by local-fields $\{J_\mu, J_\nu, \dots\}$. Since the parity transformation increases the number of qubits to the number K of interactions present in the optimization problem, the original N -qubit code-space needs to be stabilized by quasi-local three- or four-qubit stabiliz-

ers of the form $H_{\mathbf{z}} \propto \prod_{\mu=1}^l \hat{\sigma}_z^{(\mu)}$ (i.e. $l = 3, 4$), that act as energetic constraints on 2×2 plaquettes [33, 37].

Implementations of QAOA for parity encoded optimization problems rely on alternately driving the quantum spin system, prepared in the $|+\rangle^{\otimes K}$ state, with a driving Hamiltonian and the problem Hamiltonian. While the single qubit driving Hamiltonian $\hat{H}_X = \sum_\nu \hat{\sigma}_x^{(\nu)}$ remains as before, the problem Hamiltonian \hat{H}_P is now decomposed into a single qubit problem encoding $\hat{H}_Z = \sum_\nu J_\nu \hat{\sigma}_z^{(\nu)}$, and a quasi local constraint term $\hat{H}_C = \sum_{\mathbf{z}} H_{\mathbf{z}}$, where the sum runs over all 2×2 plaquettes denoted by \mathbf{z} . Alternately applying each of the Hamiltonian operators p times, QAOA thus generates states

$$|\psi(\alpha, \beta, \gamma)\rangle = \prod_{j=1}^p e^{-i\alpha_j \hat{H}_X} e^{-i\beta_j \hat{H}_Z} e^{-i\gamma_j \hat{H}_C} |+\rangle^{\otimes K}, \quad (2)$$

where variational parameters α_j, β_j , and γ_j ($j = 1, 2, \dots, p$) determine the duration of driving with $\hat{H}_X, \hat{H}_Z, \hat{H}_C$, respectively. Low-energy solutions to the original optimization problem are then determined in a quantum-classical feedback loop, where a classical computer optimizes the parameters (α, β, γ) , based on energy estimation obtained by repeated single qubit measurements in the z -direction.

The quantum spin system we have in mind consists of a regular array of trapped neutral atoms, e.g. Rubidium (^{87}Rb) atoms trapped in optical tweezers (cf. Fig. 1). Each atom realizes a qubit by encoding the qubit basis $\{|\downarrow\rangle, |\uparrow\rangle\}$ in a pair of atomic ground states (e.g. two hyperfine states). We assume the ability to locally address atoms with targeted laser light, e.g. by using spatial light modulators (SLMs) [13, 38–40]. The single particle operations \hat{H}_Z can then be implemented through AC Stark shifts from laser coupling to low-lying excited states. The driver Hamiltonian \hat{H}_X can be implemented through Raman transitions. In the following, we discuss the Rydberg implementation of the key nontrivial component, the many-body phase gate $e^{-i\gamma \hat{H}_C}$.

Four-qubit parity gate implementation– The main challenge for experimental realizations of the parity-QAOA algorithm is a direct and straightforward implementation of the four-qubit gate $U_{\mathbf{z}}(\gamma) = e^{-i\gamma H_{\mathbf{z}}}$. The operator $H_{\mathbf{z}}$ energetically separates plaquette states $|z_{\text{even}}\rangle$ with an even number of particles in the $|\downarrow\rangle$ state, from plaquette states $|z_{\text{odd}}\rangle$ with an odd number of particles in the state $|\downarrow\rangle$. The desired gate operation $U_{\mathbf{z}}(\gamma)$ thus corresponds to a four-qubit phase gate, mapping the plaquette states as follows:

$$\begin{aligned} U_{\mathbf{z}}(\gamma) |z_{\text{odd}}\rangle &= e^{i\gamma} |z_{\text{odd}}\rangle, \\ U_{\mathbf{z}}(\gamma) |z_{\text{even}}\rangle &= e^{-i\gamma} |z_{\text{even}}\rangle. \end{aligned} \quad (3)$$

We propose to implement $U_{\mathbf{z}}(\gamma)$ with an adiabatic protocol, such that each computational state acquires a controllable dynamical phase $|z\rangle \rightarrow e^{i\Phi_z} |z\rangle$, designed to match Eq. (3) for arbitrary angles γ .

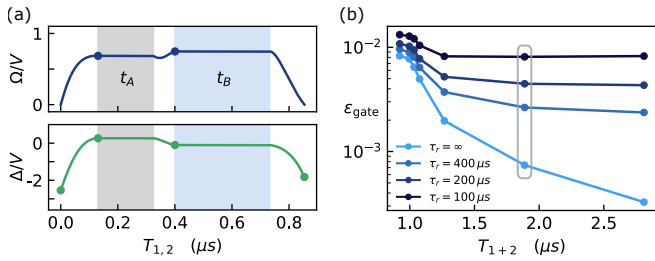


FIG. 3. (a) Two pause pulse example. Laser parameters that are used for pulse optimization are indicated as dots (see main text). (b) Gate error of the parity gate for experimental conditions as: $V = 2\pi \times 40$ MHz, $\Omega_{\max} = 2\pi \times 30$ MHz, $\Delta_{\text{start,end}}/V \in [-3.0, 0.0]$, $\Delta_{A,B}/V \in [-3.0, 1.0]$, averaged over 10^4 randomly chosen phase-combinations (see SM [36]). Highlighted points correspond to the pulse shown in panel (a), with pause-times $t_{A,B}$ adjusted to $\gamma = \pi/4$, corresponding to the maximally entangling gate operation.

the detuning at $t = 0$ and $\Omega(0) = 0$ determines to which of the eigenstates we connect when increasing $\Omega > 0$. For example, $\Delta(0) < 0$ connects us to the lowest eigenstate, and $0 < \Delta(0) < V/2$ connects to the first excited state [small arrows in Fig. 2(c)]. For illustrative purposes, we operate on the first excited many-body state. After adiabatically increasing $\Omega > 0$ and subsequently sweeping the detuning back and forth (arrows in Fig. 2), the plaquettes pick up a dynamical phase (the time integral of the particular eigenenergy-trajectory, indicated as shaded areas in Fig. 2), which is dependent on the number n , due to the many-body spectrum depending on n . We can achieve the desired effect that the odd and even plaquettes pick up equal and opposite phases $\pm\gamma$ by repeating the pulse in exactly the same fashion, but this time coupling the $|\uparrow\rangle$ ground states to the Rydberg state (panels (f) - (j) in Fig. 2). By simultaneously illuminating plaquettes that are separated by a line of non-illuminated atoms (see highlighted plaquettes in Fig. 1) to avoid crosstalk between plaquettes, the whole many-body phase gate $e^{-i\gamma\hat{H}_C}$ can be realized in 9 illumination rounds independent of system size.

Two pause protocol— We now discuss how arbitrary plaquette phases γ can be implemented using a two-pause protocol, only requiring onetime optimization and calibration of laser pulse-shapes. Our protocol relies on adiabatic trajectories $(0, \Delta_{\text{start}}) \rightarrow (\Omega_A, \Delta_A) \rightarrow (\Omega_B, \Delta_B) \rightarrow (0, \Delta_{\text{end}})$, where the corresponding laser-pulse is held (“paused”) at $(\Omega_{A,B}, \Delta_{A,B})$ for durations $t_{A,B}$ [cf. Fig. 3(a)]. The key observation is that for an arbitrary gate phase γ in Eq. (3), there exists an analytic solution of hold times $t_{A,B}$, realizing the desired phase (see SM [36]). The precise solutions, and hence the total gate duration, depend on the values of $\mathbf{\Omega} = (\Omega_A, \Omega_B)$ and $\mathbf{\Delta} = (\Delta_{\text{start}}, \Delta_A, \Delta_B, \Delta_{\text{end}})$, and the adiabatic path connecting them.

We determine the waypoints $(\mathbf{\Omega}, \mathbf{\Delta})$ of the adiabatic path by numerically optimizing the total gate duration for all values of $\gamma \in [0, 2\pi]$, for the worst case scenario,

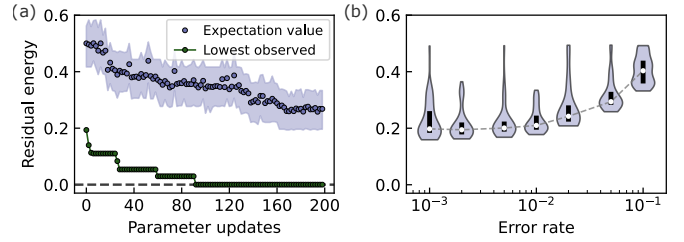


FIG. 4. (a) Example QAOA simulation for 20 qubits. Shown are the lowest observed- and average residual energy after each parameter update. (b) Distribution of average residual energies of 50 independent optimization runs (200 parameter updates) for a single optimization problem with varying error rates of the four-body parity gate. Final energy values were re-estimated via 5000 circuit executions and measurements. The black bars visualize the 25th to 75th percentiles and the white circles denote the median of the distribution.

and given experimental constraints such as achievable interaction strengths V and maximum Rabi frequencies Ω . The paths $\Omega(t), \Delta(t)$, connecting the waypoints $(\mathbf{\Omega}, \mathbf{\Delta})$, are calculated using a novel numerical approach based on quantum adiabatic brachistochrones (QAB) [41–43] (see SM [36], which includes Refs. [44–48]). Once this one-time optimization is done, executing QAOA consists of only varying the hold times $t_{A,B}$, irrespective of the precise problem.

Gate performance— We now assess the performance of our parity gate protocol for a realistic experimental scenario. We assume an interaction strength $V = 2\pi \times 40$ MHz, e.g. achievable for 68S states of ^{87}Rb , and particles spaced at $5\mu\text{m}$. In the SM [36] we provide a detailed discussion of potential considerations, including three- and four-body effects. We note that for interaction strengths of this magnitude and μs gate operation times, trapping with about $1 - 2\text{mK}$ deep traps of the Rydberg states would be required [49, 50], to minimize or prevent excitations of higher motional states in the tweezer traps and their associated fluctuations in interaction strengths, which would adversely affect gate fidelities. The lifetime of the 68S states at 300 K is about $150\mu\text{s}$ [51].

For parameters in this regime, Fig. 3(b) analyzes the average gate-error $\epsilon_{\text{gate}} = 1 - \overline{\mathcal{F}}$, where $\overline{\mathcal{F}}$ denotes the mean of the average gate fidelity over 10^4 gate realizations, i.e. γ -values. We optimized the laser-parameters in the coherent, i.e. noiseless, regime for various levels of adiabaticity using a 100-steps basin-hopping algorithm [52]. There, the gate error [see light blue line in Fig. 3(b)] solely originates from diabatic errors and thus can be arbitrarily reduced by making the gate more adiabatic, i.e. slower. However, the finite lifetime of Rydberg states restricts the maximal gate-duration and thus limits the achievable gate-performance. Including dissipation (see SM [36], which includes Refs. [53–55]) shows that the best possible gate-performance is a trade-off between diabatic and dissipative error mechanisms [see Fig. 3(b)].

QAOA simulations— We numerically demonstrate the

feasibility of our parity-QAOA implementation on small test-scale problems of $K = 20$ qubits (see Fig. 4), arranged in a 4×5 grid, with local fields J_j randomly chosen to be either -1 or 1 . This corresponds to a small example optimization problem of a bipartite graph involving 9 logical qubits. Our main objective is to investigate the robustness of our QAOA scheme under varying (depolarizing) noise levels of the four-qubit parity gate (see SM [36], which includes Refs. [56, 57]). We numerically simulated the QAOA circuit Eq. (2) with circuit depth $p = 3$ for various error rates of the four-body gate, while keeping single-qubit error rates constant at 0.05%. Figure 4(a) shows the residual energy $E_{\text{res}} = (\langle E \rangle - E_{\text{min}})/(E_{\text{max}} - E_{\text{min}})$, as function of the number of parameter updates for a sample experiment with a four-qubit error rate of 0.1%. Furthermore, Fig. 4(b) shows that the performance is robust against error rates up to a few percent, which can be achieved with sub- μs Rydberg gate protocols [cf. Fig. 3(b)].

Conclusion and Outlook—While present day Rydberg experiments have seen enormous progress in quantum state control and particle numbers, their focus has been so far predominantly on quantum simulation. Our proposed Rydberg parity gate will enable these experiments to explore solving arbitrary combinatorial optimization problems, providing a new direction towards quantum computing tasks, without requiring substantial hardware changes. We want to emphasize, that our scheme directly

relates laser-pulse hold-times to the variational QAOA parameters and thus is a prime example of hardware-algorithm co-design.

The inherent scalability of the parity architecture is naturally complemented by the scalability of the Rydberg platform. We expect intermediate scale Rydberg experiments with up to hundreds of atoms to be able to investigate parity-QAOA in regimes where it cannot be investigated by classical simulations anymore. Going beyond these system sizes, the Rydberg lifetimes will become an issue, and will require either larger interaction strengths for faster gate operations, or modified implementations suited for circular Rydberg states with much longer lifetimes [58–60].

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