Quantum Simulation and Optimization using Rydberg Atoms

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Contents

Some facts on Rydberg atoms I

Scaling with principal quantum number n

- Size $\propto n^2$
- Energies $\propto \frac{1}{n^2}$, spacing $\propto \frac{1}{n^3}, \frac{1}{n^5}$
- Lifetime $\propto n^3$ low l, $\propto n^5$ high l
- Polarizability $\propto n^7$, $C_6 \propto n^{11}$

Rydberg-ground state comparison for $n = 50$ (hydrogen, atomic units)

Size	2.5×10^3
Lifetime (low l)	1.25×10^5
Lifetime (high l)	3.1×10^8
Energy spacing Rydberg levels	8×10^{-6}
Polarizability	7.8×10^{11}

Some facts on Rydberg atoms II

Energy spectrum: $E \propto \frac{1}{(n-\delta_l)^2}$, $\delta_l(n) = \delta_{l0} + \frac{\delta_{l2}}{(n-\delta_{l0})^2}$

- Quantum defect splitted states: low-l core scattering
- High-l: defect negligible, degenerate manifold for $l > 2$, degree of degeneracy $\propto n^2$

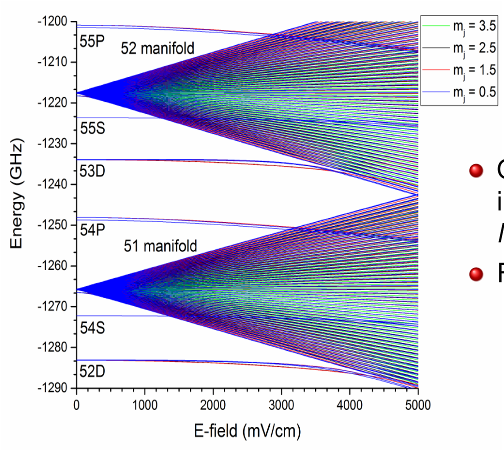
$l-$state	δ_{l0}	δ_{l2}
$ns_{1/2}$	3.13	0.178
$np_{1/2}$	2.65	0.290
$np_{3/2}$	2.64	0.295
$nd_{3/2}$	1.35	-0.603
$nd_{5/2}$	1.35	-0.596
$nf_{5/2}$	0.017	-0.085
$nf_{7/2}$	0.017	-0.087
ng	0.004	-0.018

Rubidium 85

Gallagher et al, Phys.Rev.A 67, 052502 (2003); ibid Phys.Rev.A 74, 054502 (2006)

$\Rightarrow$ Multi-Channel Quantum Defect Theory (Seaton, Greene, Sadeghpour,....)

Some facts on Rydberg atoms III



- Quantum defects: low $l-$states interdispersed into high $l-$manifolds of states
- Field sensitivity: Static B,E fields

$\Rightarrow$ Huge Rydberg-Rydberg interactions $\propto \frac{1}{r^6}, \frac{1}{r^3}$; van der Waals, resonant dipole dipole interactions

Ingredients for quantum simulation and computation

MANY-BODY RYDBERG ATOM SETUPS:

ONE OF THE MOST PROMISING PLATFORMS FOR QUANTUM SIMULATION AND QUANTUM COMPUTING

- Cooling and trapping of atoms at ultracold temperatures
- Optical tweezer technology: arbitrary geometric arrangement of traps (Kaufman and Ni , Nat.Phys.17, 1324 (2021))
- Deterministic loading eliminating defects (Endres et al, Science 354, 1024 (2016))
- Excitation to Rydberg states: long-range interactions - $C_6 \propto n^{11}$
- Many-body strongly correlated states: dipole blockade : quantum simulation (Browaeys and Lahaye, Nat.Phys. 16, 132 (2020))
- Tunable rearrangement and reconfiguration of tweezer arrays for entanglement creation $\Leftrightarrow$ Quantum gates and circuitry
- Quantum computing platform (Bluvstein et al, Nat. 626, 58 (2024))

2. Quantum Simulation of Many-Body Quantum Phases with Lattices of Rydberg Atoms

Z. Zeybek, R. Mukherjee and P.S., PRL 131, 203003 (2023)
Z. Zeybek, P.S. and R. Mukherjee, PRB 110, 075111 (2024)
Z. Zeybek, P. S. and R. Mukherjee, PRR Lett. 7, L012009 (2025)

Motivation and Problem

Interplay of short- and long-range interactions

$\Rightarrow$ Diverse phenomena with implications in particular for quantum phases in condensed matter physics

M. Bacani et al, PRB 96, 035104 (2017); f. Igloi et al, PRB 98, 184415 (2018); M. Nishino et al, PRB 100, 134414 (2019); X. Zhu et al, PRB 106, 075109 (2022)

$\Rightarrow$ Use ultracold Rydberg atoms for quantum simulation of corresponding many-body problems

M. Lewenstein et al, Adv.Phys. 56, 243 (2007); I. Bloch et al, RMP 80, 885 (2008); I. Bloch et al, Nat.Phys. 8, 267 (2012)

Optical lattice or tweezer based platforms of neutral Rydberg atoms are highly practical quantum simulators:

Tunable strong interactions ranging from dipole-dipole $\propto \frac{1}{r^3}$ to van der Waals interactions $\propto \frac{1}{r^6}$

COMBINATION THEREOF HAS RARELY BEEN INVESTIGATED, IF AT ALL.

Short and Long-Range Interactions

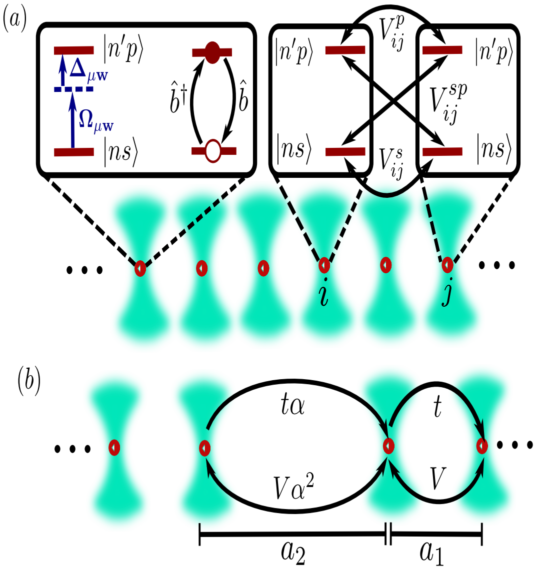
We study the combined effects of van der Waals and dipole-dipole interactions in one-dimensional uniform and dimerized lattices.

$\Rightarrow$ Novel quantum phases in the ground state encapsulating ordered and liquid phases.

Specifically, we will see that

- Uniform chain: Competing boundaries between Luttinger liquid (LL) and the gapped density wave (DW) ordered phases
- Dimerized chain: Apart from bond-order (BO) and DW phases, we find unique bond-order-density-wave (BODW) phase

Setup



- Uniform (a) and dimerized (b) chains of **two-level Rydberg states**
- Microwave laser with Rabi frequency $\Omega_{\mu w}$ and detuning $\Delta_{\mu w}$
- vdW and dipolar exchange interactions
- Dimerized chain: alternating intracell a_1 and intercell a_2 lattice constants

Rydberg Hamiltonian

$$\hat{H}_A = \sum_i \left[\frac{\Omega_{\mu w}}{2}(\hat{\sigma}_i^{sp} + \hat{\sigma}_i^{ps}) - \Delta_{\mu w}\hat{\sigma}_i^{pp}\right] + V^p \sum_{i<j} \frac{\hat{\sigma}_i^{pp}\hat{\sigma}_j^{pp}}{|i-j|^6}$$
$$+ V^s \sum_{i<j} \frac{\hat{\sigma}_i^{ss}\hat{\sigma}_j^{ss}}{|i-j|^6} + V^{sp} \sum_{i<j} \left(\frac{\hat{\sigma}_i^{sp}\hat{\sigma}_j^{ps}}{|i-j|^3} + \text{h.c.}\right)$$

$\hat{\sigma}_i^{\alpha\beta} = |\alpha\rangle_i \langle\beta|$ is the projection operator to the relevant atomic state.

$\alpha, \beta \in \{|ns\rangle, |n'p\rangle\}$ at site i.

$V^p = C_6^p/a^6$ and $V^s = C_6^s/a^6$ are vdW interactions.

$V^{sp} = C_3/a^3$ dipole-dipole interaction strength.

Mapping to extended Bose-Hubbard Hamiltonian

$$\hat{H}_{eBH} = \sum_{i<j} t_{ij}(\hat{b}_i^\dagger \hat{b}_j + \text{h.c.}) + \sum_{i<j} V_{ij}\hat{n}_i\hat{n}_j - \sum_i(\Delta_{\mu w} + \mathcal{I}_i)\hat{n}_i + \frac{\Omega_{\mu w}}{2}\sum_i(\hat{b}_i^\dagger + \hat{b}_i)$$

Occupation of state $|n'p\rangle$ at site i is associated with the presence of a boson at that site: presence $|\bullet\rangle_i$ versus absence $|\circ\rangle_i$ of a boson which implies the occupation of state $|ns\rangle$.

Arbitrary state $|ns\ n'p\ n'p\ ns\ldots\rangle \Leftrightarrow |\circ\bullet\bullet\circ\ldots\rangle$.

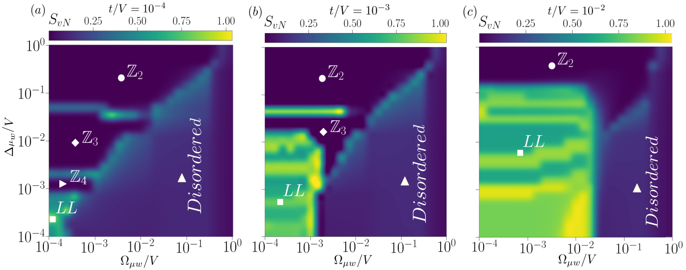
Hard-core constraint. $\hat{b}^\dagger(\hat{b})$ - bosonic creation (annihilation) operator.

Mapping $\hat{\sigma}^{ps} \rightarrow \hat{b}^\dagger$, $\hat{\sigma}^{pp} \rightarrow \hat{n} = \hat{b}^\dagger\hat{b}$ and $\hat{\sigma}^{ss} \rightarrow (\mathbf{1} - \hat{n})$ with $(\hat{b}_i^\dagger)^2 = 0$.

Chemical potential $(\Delta_{\mu w} + \mathcal{I}_i)$

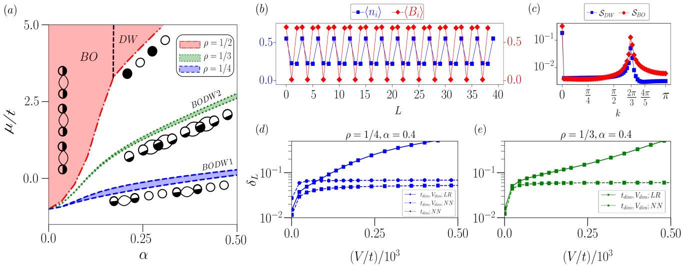
Peculiarities: Long-range hopping and interactions as well as breaking of U(1) symmetry $\Rightarrow$ number of bosons is not conserved.

Ground state phase diagram: Uniform lattice

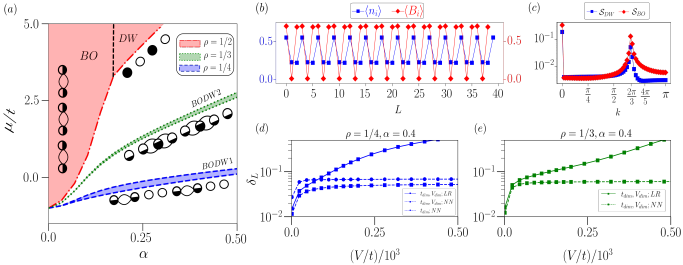


- Phase diagrams showing the ground-state entanglement entropy S_{vN} of $\hat{H}_{eBH}$ in the $(\Delta_{\mu w}, \Omega_{\mu w})$ parameter space with varying t/V in (a), (b) and (c) respectively.
- Vanishing S_{vN} (dark blue): gapped ordered phases $Z_{q=2,3,4}$.
- Yellow-green regions: finite S_{vN} - gapless Luttinger liquid (LL) phase.

Ground state phase diagram: Dimerized lattice



- (a) Gapped phases of $\hat{H}_{dim}$ as a function of $\alpha = (\frac{a_1}{a_2})^3$ with fixed $V/t = 200$.
- Red dashed-dotted line: lower boundary at $\rho = 1/2$.
- Green dotted and the blue dashed lines: boundaries of the BODW phases at $\rho = 1/3$ and $\rho = 1/4$.
- Density and bond formation in each phase are symbolically represented.
- BODW phases are a cumulative effect of (i) long-range repulsive interactions (ii) large α (iii) sharing bosons due to constraint of filling factors.



- (b) Expectation values of the bond energy (red, diamond) and density (blue, square) operators for the BODW phase at $\rho = 1/3$ for $\alpha = 0.4$ and $V/t = 200$. Bond energy operator $\hat{B}_i = \hat{b}_i^\dagger \hat{b}_{i+1} + \text{h.c.}$
- Corresponding structure factors in (c): $\mathcal{S}_{BO}(k) = (1/L^2) \sum_{i,j} e^{ikr} < \hat{B}_i \hat{B}_j >$ and $\mathcal{S}_{DW}(k) = (1/L^2) \sum_{i,j} e^{ikr} < \hat{n}_i \hat{n}_j >$.
- (d,e) Figure comparing the gap δ_L for BODW phases at filling $\rho = 1/4$ and $\rho = 1/3$ with different types of couplings.

Future perspectives...

- Higher dimensions: 2D, 3D lattices
- Different crystalline or aperiodic structures
- Quench dynamics across phase boundaries

3. An Efficient Quantum Algorithm Solving the Integer Programming Optimization Problem

K. Goswami, P.S. and R. Mukherjee, arXiv:2508.13906

Relevance of Optimization Problems

OPTIMIZATION PROBLEMS:

LOGISTIC OPERATIONS

BANK PORTFOLIO

Here: An Algorithm with Exponential Reduction in Time Complexity

AIRCREW AIRCRAFT ASSIGNMENT

FEEDSTOCK SELECTION

- Very difficult task to solve combinatorial optimization problems classically: NP-hard problems

  R.M. Karp, On the computational complexity of combinatorial problems, Wiley New York 1975

- Quantum and quantum-inspired algorithms as an alternative: efficiency of resources and time

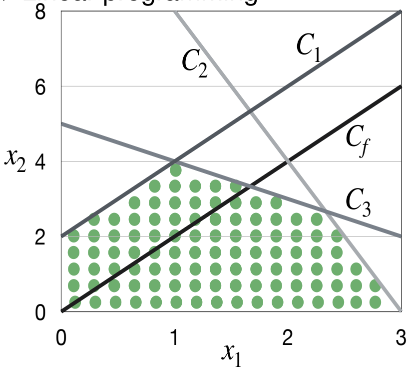
Integer Programming Problem

Definition: Optimize $C(x_1, ..., x_n)$ with $x_i \in \{..., -1, 0, +1, ...\}$ under the constraints $C_1(x_i, ..., x_j)$, $C_2(x_p, ..., x_q)$, ...

NP HARD PROBLEM !

Bottleneck in solving: INTEGER values

- Variables: Integer ⇒ Continuous
- Problem: Integer programming ⇒ Linear programming
- Complexity: NP hard ⇒ P



IP Problem: Quantum approach so far

- Variables: Integer ⇒ Binary (all of them)
- Problem: Integer programming ⇒ QUBO (most of them)
- Scaling: 8 variable + 4 constraints ⇒ 250 variables
- Extra variable to make the problem unconstrained
- No direct method available for encoding

Very expensive in resources ... no direct mapping !

C.Y. Chang et al, **On hybrid quantum and classical computing algorithms for mixed integer programming**, arxiv:2010.07852 (2020)
S. Okada et al, **Efficient partition of integer optimization problems with one-hot encodings**, Scient.Rep. 9, 13036 (2019)
M. Svensson et al, **Hybrid quantum classical heuristic to solve large scale integer linear programs**, Phys.Rev.Appl. 20, 034062 (2023)
F. Khosravi et al, **Mixed integer programming using a bosonic quantum computer**, IEEE QCE 1, 184 (2023).

Birds eye view of our algorithm: Step 1

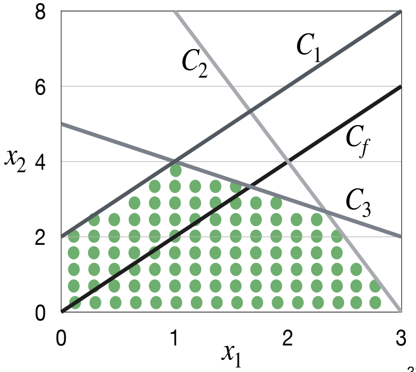
IMPLEMENTING THE CONSTRAINTS:

Via **filtering process** - quantum operations lead to

Separation of states: **Feasible** and **infeasible** region

Amplitude amplification and measurement

⇒ **Projection on feasible states**



Birds eye view of our algorithm: Step 2

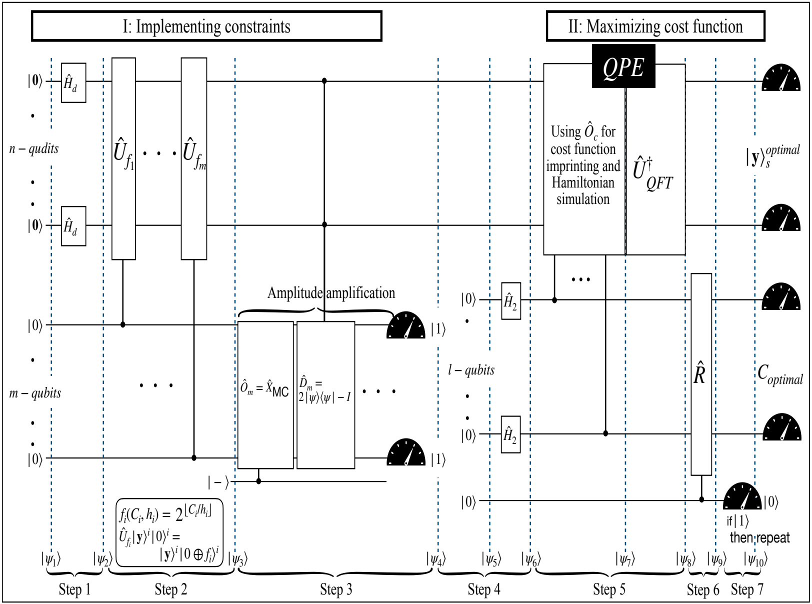
Integer variables as qudits:

Each constraint has a qubit $(0/1)$

Maximize the cost function: Cost function imprinting via quantum operations $\Rightarrow$ Cost function stored in the quantum state

Single qubit rotation and measurement: **highest probability for the optimal solution**

Quantum Circuit



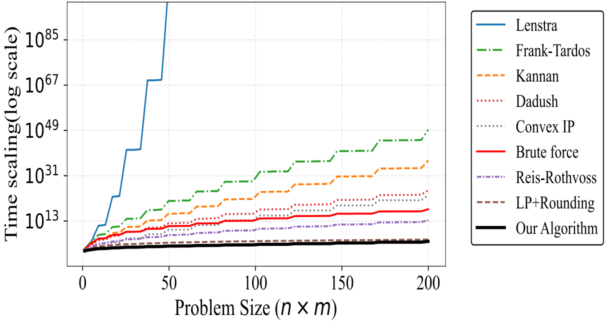
Comparison with classical algorithms

Exponential gain !!!

Our Algorithm works for **any IP** with time scaling $\mathbf{T_Q \sim mn^2 \log d + 6 \cdot d^{n/2} + n\epsilon_{QPE}^{-1}}$ to give **exact** solutions				
Class	**Method**	**Time Scaling T_{Cl}**	**Type**	**Speed-up criterion of our algorithm $T_{Cl}/T_Q > 1$**
Linear IP	Lenstra (1983)	$2^{n^3} \cdot m^3 \log^2 V$	Exact	$\sim 2^{n^3}/d^{n/2}$: Speed-up for $n \geq \sqrt{\log \sqrt{d}}$
Linear IP	Kannan (1987)	$n^{2n} e^{O(n)} \cdot m^2 \log^2 V$	Exact	$\sim n^{2n} \cdot e^{O(n)}/d^{n/2}$: Speed-up for $n > (d/e^{O(1)})^{1/4}$
Linear IP	Frank-Tardos (1986)	$n^{2.5n} \cdot 2^{2n} \cdot m^2 \log^2 V$	Exact	$\sim n^{2.5n} \cdot 2^{2n}/d^{n/2}$: Speed-up for $n > (d/4)^{1/5}$
Linear IP	Dadush (2011)	$n^n \cdot 2^n \cdot m^2 \log^2 V$	Exact	$\sim n^n \cdot 2^n/d^{n/2}$: Speed-up for $n > \sqrt{d/4}$
Linear IP	Reis-Rothvoß (2023)	$(\log n)^{3n} \cdot m^4 \log^3 V$	Exact	$\sim \log n^{3n}/d^{n/2}$: Speed-up for $n > e^{d^{1/6}}$
Convex IP	Convex IP (fixed dim)	$(n \log V)^{2n} \cdot m^3$	Exact	$\sim n^{2n}/d^{n/2}$: Speed-up for $n > d^{1/4}$
Any IP	Brute force	$d^n \cdot m \cdot n^k \cdot \log^c L$	Exact	$d^{n/2}$: Speed-up for all n
Linear IP	LP + Rounding	$m^{3.5} n^2 \log^2 V$	**Approximate**	Speed up only for small d and small n, $d < n^{4/n}$
General non-linear IP[a]	Heuristics	Undecidable/EXP-hard	–	Always (no efficient classical algorithm)[b]

[a] There are algorithms for convex non-linear IP with scaling $\sim n^{2n}$ and no algorithm with provable time complexity for a general non-convex NLIP [60].

[b] Our algorithm incurs a speed-up when the problem instance is decidable, while for undecidable instances, a set of finite measurements of the qubits in the constraint register can effectively provide the information. Refer to the Results section for further explanation.



Key Highlights

- **Direct integer $\Rightarrow$ Qudit encoding**
- **Scalable multi qudit circuit**
- **Three step pipeline:**
  1. Distillation $\rightarrow$ filters infeasible regions
  2. Phase/amplitude encoding $\Rightarrow$ encodes cost function
  3. QPE + rotation $\rightarrow$ amplifies optimal solution probability
- **Provable guarantee:** optimal solution has **highest measurement probability**
- **Quantum advantage in runtime: Exponential reduction in time complexity**
  $O(d^{n/2} + mn^2 logd + \frac{n}{\epsilon_{QPE}})$ vs. $O(d^n)$ in the classical case
- **Works for linear and nonlinear IP problems with provable advantage**

Conclusions

- Qudit approach is a key element
- Exponential reduction also due to the two registers: first the feasible space is determined and then imprinted on the qudit solution space
- Our IP approach with a modular structure could be of more general use: whereever there is a dividing of the solution space...
- Existing hardware: Ions, SC Qubits, Photonic,..., but in particular: Rydberg tweezer platform: Natural Qudit structure.

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Thank you very much for your attention!