

Hubbard physics with Rydberg atoms: Using a quantum spin simulator to simulate strong fermionic correlations

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We propose a hybrid quantum-classical method to investigate the equilibrium physics and the dynamics of strongly correlated fermionic models with spin-based quantum processors. Our proposal avoids the usual pitfalls of fermion-to-spin mappings thanks to a slave-spin method which allows to approximate the original Hamiltonian into a sum of self-correlated free fermions and spin Hamiltonians. Taking as an example a Rydberg-based analog quantum processor to solve the interacting spin model, we avoid the challenges of variational algorithms or Trotterization methods. We explore the robustness of the method to experimental imperfections by applying it to the half-filled, single-orbital Hubbard model on the square lattice in and out of equilibrium. We show, through realistic numerical simulations of current Rydberg processors, that the method yields quantitatively viable results even in the presence of imperfections: it allows to gain insights into equilibrium Mott physics as well as the dynamics under interaction quenches. This method thus paves the way to the investigation of physical regimes, whether out of equilibrium, doped, or multiorbital, that are difficult to explore with classical processors.

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I. INTRODUCTION

Decades of theoretical efforts have led to tremendous progress in the understanding of the exotic phases of strongly correlated electron systems. For instance, lots is known about the physics of their minimal model, the Hubbard model [1,2]. Yet, the exponential difficulty of the underlying many-body problem still poses formidable challenges in low-temperature, doped phases relevant to cuprate superconductors, in multiorbital settings relevant, for instance, to iron-based superconductors [3] and the recent Moiré superconductors [4], or in out-of-equilibrium situations like sudden quenches that lead to a fast growth of entanglement [5].

Quantum processors, i.e., controllable, synthetic quantum many-body systems [6], are promising to solve these outstanding challenges [7]. Ultracold fermionic atoms trapped in optical lattices were already implemented more than a decade ago [8–17] as the most direct, or “analog,” quantum processors of fermions. They allowed to observe signatures of, for instance, Mott physics, while operating, so far, at temperatures too high to gain insights into pseudogap or superconducting phases.

In contrast, universal “digital” quantum processors rely on quantum bits encoded on two-level or “spin- $\frac{1}{2}$ ” systems, and operate logic gates on them. They in principle enable the simulation of the second-quantized fermionic problems explored in materials science [18] or chemistry [19]. Yet,

early attempts are facing the physical limitations of these processors in terms of the number of qubits and number of gates that can be reliably executed before decoherence sets in. Fermionic systems are particularly demanding due to the loss of locality of the Hamiltonian [20,21] or the need for auxiliary qubits [22–24] that come with translating to a qubit language. Both constraints generically lead to longer quantum programs, and hence an increased sensitivity to imperfections. To alleviate those issues, hybrid quantum-classical methods [25,26] such as the variational quantum eigensolver (VQE, [27]) were proposed, with many developments but without clear-cut advantage so far.

Despite remarkable recent progress towards large-size digital quantum processors, “analog” quantum processors remain a serious alternative to explore fermionic problems. Beyond the aforementioned ultracold atoms, analog platforms include systems of trapped ions and cold Rydberg atoms. The lesser degree of control of these processors, with a fixed, specific “resource” Hamiltonian that does not necessarily match the “target” Hamiltonian of interest, is compensated for by the large number of particles that can be controlled, with now up to a few hundreds of particles [28–30]. In addition, the parameters of the resource Hamiltonian are usually precisely controlled in time [28,31–35]. This has enabled the use of such processors to study many-body problems in several recent works [34–38]. For instance, [36] have investigated the physics of the Schwinger model, a toy problem for lattice quantum electrodynamics, by leveraging the similarity between the symmetries of a 20-ion quantum simulator and those of the Schwinger model.

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However, finding such a similarity between target and resource Hamiltonian is rare. For instance, the question of how to tackle a fermionic many-body problem with a spin-based, analog simulator is an open problem.

In this paper, we propose a method to address this problem considering a specific processor, namely, an analog Rydberg quantum processor [33,39]. By using a self-consistent mapping between the fermionic problem and a “slave-spin” model, we circumvent the nonlocality issues related to fermion-to-spin transformations. We show that the method allows one to compute key properties of the Hubbard model in and out of equilibrium. We show, through realistic numerical simulations, that it does so even in the presence of hardware imperfections like decoherence, readout error, and finite-sampling shot noise.

II. THEORY

A. The slave-spin method

As a proof of concept, we consider the single-band, half-filled Fermi-Hubbard model on a square lattice. Its Hamiltonian,

$$H_{\text{Hubbard}} = \sum_{i,j,\sigma} t_{ij} d_{i\sigma}^\dagger d_{j\sigma} + \frac{U}{2} \sum_i (n_i^d - 1)^2, \quad (1)$$

contains creation (respectively annihilation) operators $d_{i\sigma}^\dagger$ (respectively $d_{i\sigma}$) that create (respectively annihilate) an electron of spin σ on lattice site i , with a hopping amplitude t_{ij} between two sites (we will focus on nearest-neighbor hopping only, $t_{ij} = -t\delta_{(ij)}$) and an onsite interaction U . The chemical potential was set to $\mu = U/2$ to enforce half-filling.

This prototypical model of strongly correlated electrons is hard to solve on classical processors [40], especially in out-of-equilibrium situations where the most advanced methods are usually limited to short-time dynamics. Instead of directly tackling this fermionic model, we thus resort to a separation of variables that singles out two degrees of freedom of the model, namely, spin and charge. This is achieved by resorting to a “slave-particle” method known as Z_2 slave-spin theory [41]. We replace the fermionic operator $d_{i\sigma}^\dagger$ by the product of a pseudofermion operator $f_{i\sigma}^\dagger$ and an auxiliary spin operator S_i^z ($S_i^{a=x,y,z}$ denote the Pauli spin operators), namely, $d_{i\sigma}^\dagger = S_i^z f_{i\sigma}^\dagger$. The ensuing enlargement of the Hilbert space is compensated for by imposing constraints $S_i^z + 1 = 2(n_i^f - 1)^2$ on each site. In our case, namely the single-orbital, half-filled Hubbard model on a square, i.e., bipartite, lattice, particle-hole symmetry holds, which is a sufficient condition for the constraint to be automatically satisfied [42].

We then perform a mean-field decoupling of the pseudofermion and spin degrees of freedom $S_i^z S_j^z f_{i,\sigma}^\dagger f_{j,\sigma} \approx \langle S_i^z S_j^z \rangle f_{i,\sigma}^\dagger f_{j,\sigma} + S_i^z S_j^z \langle f_{i,\sigma}^\dagger f_{j,\sigma} \rangle - \langle S_i^z S_j^z \rangle \langle f_{i,\sigma}^\dagger f_{j,\sigma} \rangle$. We obtain a sum of two self-consistent Hamiltonians $H \approx H_f + H_s$:

$$H_f = \sum_{i,j,\sigma} Q_{ij} f_{i,\sigma}^\dagger f_{j,\sigma}, \quad (2a)$$

$$H_s = \sum_{i,j} J_{ij} S_i^z S_j^z + \frac{U}{4} \sum_i S_i^x, \quad (2b)$$

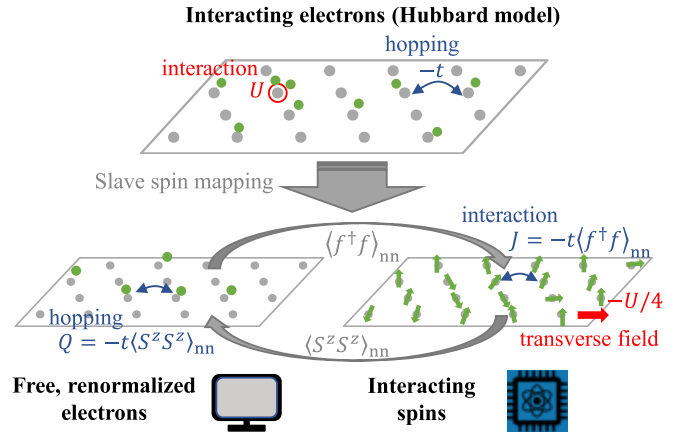


FIG. 1. Slave-spin mapping. The Hubbard Hamiltonian (top) is mapped onto two self-consistently determined simpler problems: an efficiently solvable free-fermionic Hamiltonian with a renormalized hopping [bottom left, $H_f(Q)$ in the text], and a transverse-field Ising Hamiltonian [bottom right, $H_s(J)$ in the text], which we solve using a Rydberg-based quantum processor.

with $Q_{ij} = t_{ij} \langle S_i^z S_j^z \rangle$ and $J_{ij} = \sum_{\sigma} t_{ij} \langle f_{i,\sigma}^\dagger f_{j,\sigma} \rangle$. In our particle-hole symmetric model, the constraint will be automatically fulfilled at the mean-field level [43,44].

Solving the Hubbard model using slave-spin theory amounts to solving these two self-consistently defined Hamiltonians. This is done iteratively, as illustrated in Fig. 1. We start from an initial guess for the renormalized hopping Q to initiate the self-consistent computation. First, we calculate on a classical processor the correlation function $\langle f_{i,\sigma}^\dagger f_{j,\sigma} \rangle$ of the pseudofermion problem, needed to define the spin interaction J_{ij} . The full derivation can be found in the Supplemental Material [45], Sec. II A (see also Refs. [46–50] therein). Second, as the spin problem is hard to solve on a classical processor, we use the analog quantum processor to compute its spin-spin correlation function. Since H_s is of infinite size, we first reduce it to a finite-size problem by using a cluster mean-field approximation, as done in, e.g., [51] we solve

$$H_s^C = \sum_{i,j \in C} J_{ij} S_i^z S_j^z + \frac{U}{4} \sum_{i \in C} S_i^x + \sum_{i \in C} h_i S_i^z, \quad (3)$$

where C denotes the set of N cluster sites and $h_i = 2z_i \bar{m}$ is the self-consistent mean field that mimics the influence of the infinite lattice. Here, z_i is the number of neighbors of site i outside the cluster, $\bar{J} = \frac{1}{N_p} \sum_{(i,j) \in C} J_{i,j}$ is the average nearest-neighbor coupling (N_p is the number of nearest-neighbor links inside the cluster), and $\bar{m} = \frac{1}{N} \sum_{i \in C} \langle S_i^z \rangle$ is the average magnetization. This model needs to be solved iteratively by starting from a guess for the mean field \bar{m} . For a given value of this mean field, the finite spin problem defined by H_s^C is solved using a quantum algorithm (described below). This yields the correlation function $\langle S_i^z S_j^z \rangle$ and closes the self-consistent loop, which runs until convergence. At convergence, we extract relevant observables of the original Hubbard model. For instance, the quasiparticle weight Z of the original model, which measures the quantum coherence of the fermionic excitations, is obtained via the spin model’s magnetization: $Z = \bar{m}^2$ (we

also have access to site-resolved magnetizations (S_i^z) and hence site-resolved quasiparticle weights).

B. Quantum algorithm for the spin Hamiltonian

Let us turn to the solution of the (cluster) spin problem H_s^C . It is nothing but the transverse-field Ising model, which could be a candidate problem for reaching quantum advantage using gate-based quantum processors [52]. As it turns out, its form is similar to the Hamiltonian realized experimentally by Rydberg atoms trapped with optical tweezers, for which the geometry of the array can be chosen at will [33]:

$$\hat{H}_{\text{Rydberg}} = \sum_{i \neq j} \frac{C_6}{|\mathbf{r}_i - \mathbf{r}_j|^6} \hat{n}_i \hat{n}_j + \frac{\hbar \Omega(\tau)}{2} \sum_i \hat{S}_i^x - \hbar \delta(\tau) \sum_i \hat{n}_i, \quad (4)$$

where $\Omega(\tau)$ and $\delta(\tau)$ are the time-dependent Rabi frequency and laser detuning, and C_6 the magnitude of the interatomic van der Waals interactions; $\hat{n}_i = (I_i + S_i^z)/2$. Therefore, we can make use of the Rydberg processor to attain the ground state of H_s^C using an annealing procedure:¹ we start from drive parameters $\Omega(\tau = 0) = 0$ and a large positive $\delta(\tau = 0)$ so that the system's native initial state $|\psi_{\text{start}}\rangle = |g\rangle^{\otimes N}$ is the ground state of the initial Hamiltonian. We then, for a long enough annealing time, ramp the Rabi frequency and detuning to reach the final values $\hbar \Omega(\tau_{\text{max}}) = \frac{U}{2}$, $\hbar \delta(\tau_{\text{max}}) = \sum_{j \neq i} \frac{C_6}{r_{i,j}^6} - 4\bar{J}mz_i$. Optimizing the atom positions in such a way that $\frac{C_6}{r_{i,j}^6} \approx 4J_{i,j}$ (details about this optimization are in the Supplemental Material [45], Sec. III A), the final Hamiltonian will be H_s^C . Hence, following the adiabatic theorem, the procedure should (approximately) bring the system to the ground state of H_s^C . We can finally measure the spin-spin correlation function on this state.

III. RESULTS

A. Results at equilibrium

We implemented this self-consistent procedure with a realistic numerical simulation of a Rydberg atom processor. We repeated the computation for several values of the local Hubbard interaction U to obtain the evolution of the quasiparticle weight Z as a function of U , as shown in Fig. 2, for cluster sizes, and hence number of atoms, of 4, 6, 8, and 12. Aside from the shot noise, intrinsic to any processor due to the measurement process (the number of measurement is noted N_s), the main experimental limitations were considered in order to account for the true potential of current processors: dephasing noise (with a strength γ), measurement error (characterized by a percentage ϵ), global detuning, finite annealing times

¹The main difference between \hat{H}_{Rydberg} and H_s^C is the sign of the interaction: it is positive for Rydberg atoms, negative (since usually $t_{ij} < 0$) for the slave-spin problem. Thus, in practice, parameters are tuned such that the annealing procedure is performed from an initial Hamiltonian of which the system's initial state is its most excited state to the final Hamiltonian $-H_s^C$. The adiabatic theorem can also be applied for the most excited state and therefore the procedure should bring the system to (approximately) the most excited state of $-H_s^C$, i.e., the ground state of H_s^C .

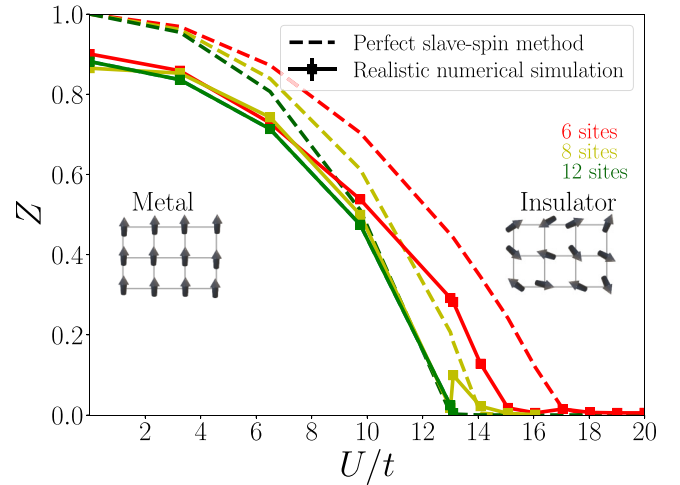


FIG. 2. Mott transition observed with the slave-spin method on a realistic numerical simulation of Rydberg atoms processor. The characteristics of the processor considered are $\tau_{\text{max}} = 4 \mu\text{s}$, $\gamma = 0.02 \text{ MHz}$, $N_s = 150$, $\epsilon = \epsilon' = 3\%$, and 5×5 loops allowed (see Supplemental Material, Sec. III C [45]). The error bar is the standard error stemming from ϵ and N_s .

τ_{max} , and imperfect positioning of the atoms to reproduce the right magnetic coupling (see Supplemental Material [45], Sec. III C, for more details). Despite these limitations, leading to few points being far from the noiseless result due to error accumulation, the quasiparticle weight we obtain (solid lines) is in fair agreement with the one obtained from a noiseless solution without shot noise of the spin model (dashed lines). The Rydberg processor can thus be used to get a reasonable estimate of the Mott transition, i.e., the value U_c when Z vanishes and the system turns Mott insulating. While for the half-filled, single-band model studied in this proof-of-concept example, classical methods can be implemented to efficiently solve the spin model (see, e.g., [53]), other regimes are less readily amenable to a controlled classical computation: doped regimes, multiorbital models, and dynamical regimes. We investigate the latter regime in the next paragraph.

B. Results out of equilibrium

We thus turn to a dynamical setting to emphasize the potential advantage brought by the use of quantum processors in this slave-spin framework. Starting from a noninteracting ground state ($U = 0 \text{ MHz}$), we suddenly switch on the value of the local interaction to a final value U_f . Our goal is to validate that the method implemented on a realistic quantum processor recovers the phenomenology observed in previous experimental and theoretical studies of quenched Hubbard systems [42,43,54–61], such as the collapse and revival oscillations of various observables in the $U_f \gg U_c$ regime, with a $2\pi/U_f$ period, and a damping that increases with bandwidth. In the $U_f \ll U_c$ regime, overdamped oscillations have been observed (see [58] for instance).

Here, we look for this phenomenology in the time evolution of the quasiparticle weight Z . Within the slave-spin method applied to the single-site Hubbard model at half-filling, interaction quenches are simple to implement:

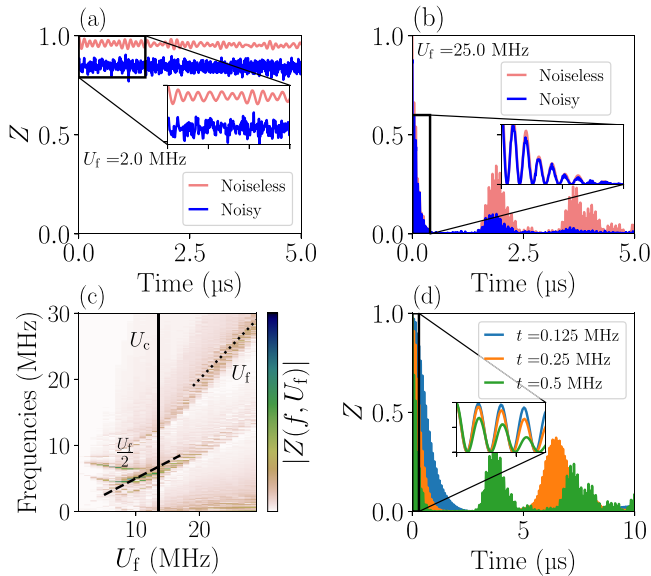


FIG. 3. Dynamical response of the quasiparticle weight after an interaction quench. $N = 12$ spin cluster. Time evolution of Z for (a) $U_f = 2$ MHz and (b) $U_f = 25$ MHz. The red line shows the noiseless annealing solution and the blue line a realistic numerical simulation on Rydberg atoms processor ($\gamma = 0.02$ MHz, $\epsilon = \epsilon' = 3\%$, $N_s = 150$ shots, realistic Ising interactions and a global detuning are imposed). (c) Fourier transform amplitude $|Z(f, U_f)|$. The vertical black line shows the equilibrium critical value U_c as computed from Fig. 2. (d) Impact of the hopping terms t on the damping of the response of Z after a quench ($U_f = 13 \approx U_c$). The blue, orange, and green lines represent the result for $t = 0.125, 0.25,$ and 0.5 MHz, respectively.

translation invariance on the lattice makes the dynamics of pseudofermions trivial when starting from an eigenstate (see [42] and the Supplemental Material [45], Sec. I D). Thus, only the dynamics of the spin model are of interest: the procedure boils down to quenching the value of the transverse field in Eq. (3) from 0 to $U_f/4$. On the Rydberg processor considered here, this means switching the Rabi frequency from zero up to the desired value to obtain U_f . In practice, however, the switch-on time is not instantaneous due to the finite temporal response of the optical modulators (about 50 ns to switch from 0 MHz to $U_f = 2$ MHz): we include this effect in our calculations. One then directly measures $\langle S_z^i \rangle$ for different evolution times. In Fig. 3, we show the oscillations observed numerically for a cluster of 12 sites, with and without including the noise. The upper panels present the oscillation of Z as a function of time after a quench to $U_f = 13$ MHz (a) and to $U_f = 25$ MHz (b). From Fig. 2, we know that the phase transition for such a cluster is $U_c \approx 13.5$ MHz. In the case of $U_f = 25$ MHz ($U_f \gg U_c$), we observe the damped oscillations, both in the noiseless and the noisy settings. Because of the dephasing noise present in the experiment and included in the simulation, the agreement between the noiseless and noisy curves worsens with time. However, during the first microseconds of observations, we recover a nearly perfect oscillation from which we can extract the frequency [insets in Figs. 3(a) and 3(b)]. For $U_f = 13$ MHz ($U_f \approx U_c$), we see that Z quickly reaches a value ≈ 0.1 (slightly higher than the Z obtained for

this value of U at equilibrium), around which it oscillates. Figure 3(c) exhibits the Fourier transform of $Z(\tau)$ for various U_f for the exact slave-spin method (namely, with an exact solution of the spin model). For $U_f < U_c$, components at $\omega = U_f/2$ can be identified along with other contributions, while for $U_f > U_c$, the component at $\omega = U_f$ dominates the spectrum. This is expected from the physics of the Mott transition in the Hubbard model: above the transition, the single-particle spectrum displays a Mott gap of U_f , while below it excitations between the quasiparticle band and the emerging Hubbard bands (with energy $U_f/2$), and within the quasiparticle band, are possible. Finally, Fig. 3(d) confirms the expected increase of the damping of oscillations with the hopping strength t .

IV. CONCLUSION

In conclusion, we introduced a hybrid quantum-classical method that does not suffer from the usual overheads of translating fermionic problems to spin problems, namely, long quantum evolutions (due to nonlocal spin terms) or auxiliary quantum degrees of freedom. This is made possible by using a slave-spin mapping that turns the difficult fermionic problem into a free, and thus efficiently tractable, fermion problem that is self-consistently coupled to an interacting, yet *local*, spin problem.

Here, to solve the spin problem, we considered an *analog* Rydberg-based quantum processor that naturally implements the effective transverse-field Ising spin Hamiltonian appearing in the slave-spin approach. Its analog character allows one to circumvent the issues associated with gate-based algorithms, like Trotterization when performing time evolution, and the annealing algorithm proposed here avoids the pitfalls of today's widespread variational algorithms like VQE or its temporal counterparts. With the large number of Rydberg atoms that can be controlled in current experiments, this original approach could help tackling problems of (cluster) sizes unreachable to classical computers, without suffering from the limitations that have been pointed out [62–65] in a recent quantum-advantage experimental claim [52]: the atoms can be placed in a two-dimensional array that has high connectivity compared to the quasi-one-dimensional connectivity of the experiments, making tensor network approaches difficult [62], and the correlation lengths that can be attained experimentally in a similar context (up to 7 lattice sites, [28], i.e., 49 spins) also raise the bar for approaches that rely on a smaller effective size [63–65]. This proposal calls for further investigations. An important step would be an experimental validation with larger atom numbers than the 12 atoms we simulated here. Other improvements involve the slave-spin method itself: doped regimes (relevant to cuprate materials), multiorbital models [66] (relevant to iron-based superconductors, where orbital-selective effects may appear [67]) pose various technical difficulties that warrant further theoretical developments. In particular, the fulfillment of the constraint to ensure the states remain in the physical subspace becomes more difficult in these regimes than in the half-filled, single-band case that we studied here. Going beyond the mean-field decoupling of the pseudofermion and spin variables is also another interesting avenue.

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