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Benchmarking the Magnus Expansion for Interaction Quenches in the Fermi-Hubbard Model: Exact Diagonalization on Small Clusters

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Abstract

We investigate the nonequilibrium relaxation dynamics of the one-dimensional (1D) Fermi-Hubbard model subjected to abrupt, global interaction quenches. Specifically, we benchmark the convergence properties, structural accuracy, and algorithmic breakdown of the Magnus expansion against numerically exact results obtained via full Exact Diagonalization (ED) on small, periodic lattice clusters. By tracking the real-time evolution of local observables, double occupancy (doublon density), and many-body state fidelity metrics, we map out the validity bounds of the low-order Magnus series across weak, moderate, and strong interaction regimes. Our findings demonstrate that while the Magnus expansion provides an exceptionally accurate description of short-time coherent dynamics, rapid phase matching, and initial prethermalization tendencies, its convergence is fundamentally bottlenecked at longer timescales. This breakdown is driven by the rapid growth of multi-particle entanglement, non-local operator spreading via nested commutators, and the emergence of severe state-space fragmentation inherent to dense, strongly interacting many-body spectra.

Keywords: Nonequilibrium dynamics, Fermi-Hubbard model, Magnus expansion, Exact diagonalization, Quantum quench, Quantum thermalization.

INTRODUCTION

Understanding the real-time dynamics of isolated quantum many-body systems far from equilibrium remains one of the most fundamental challenges in modern condensed matter physics, quantum statistical mechanics, and quantum information science. Unlike classical systems, where thermalization is often attributed to stochastic interactions with an external environment, closed quantum systems evolve according to unitary dynamics and preserve the purity of the global wavefunction. Nevertheless, numerous theoretical and experimental studies have demonstrated that local observables can relax toward stationary values that closely resemble those predicted by equilibrium statistical mechanics. Explaining the microscopic mechanisms responsible for this apparent emergence of thermodynamics from reversible quantum dynamics has become a central theme in nonequilibrium quantum physics (Bukov *et al.,* 2016; Lerose & Pappalardi, 2020; Ueda, 2020).

Recent advances have further strengthened the view that quantum thermalization is intimately connected to entanglement generation, operator spreading, and the Eigenstate Thermalization Hypothesis (ETH). In generic nonintegrable systems, information initially encoded in local degrees of freedom becomes distributed across increasingly complex many-body correlations, causing subsystems to lose memory of their initial conditions and approach thermal equilibrium. Contemporary studies have highlighted the role of entanglement structure, eigenstate correlations, and quantum chaos in governing equilibration processes, while also revealing scenarios in which thermalization can be delayed, modified, or entirely suppressed by conservation laws, integrability, kinetic constraints, or emergent dynamical symmetries. Recent theoretical developments continue to refine the connection between

ETH, information scrambling, and quantum relaxation in strongly interacting many-body systems (Hahn *et al.,* 2024; Buča, 2023).

Experimentally, the development of programmable quantum simulators has transformed the study of nonequilibrium quantum matter. Ultracold bosonic and fermionic atoms trapped in optical lattices provide exceptionally clean realizations of strongly correlated lattice Hamiltonians with tunable interactions, negligible environmental coupling, and single-site measurement capabilities. These platforms have enabled direct observation of quantum transport, prethermalization, dynamical phase transitions, correlation spreading, and relaxation phenomena that were previously inaccessible in solid-state systems. Modern experiments can now track the evolution of many-body states with unprecedented temporal and spatial resolution, establishing optical lattice systems as a premier laboratory for investigating quantum thermalization and far-from-equilibrium dynamics (Trotzky *et al.,* 2012; Scherg *et al.,* 2021; Ueda, 2020). Recent progress in ultracold atomic systems continues to uncover novel dynamical regimes, including nonthermal fixed points, long-range interaction effects, and interaction-driven instabilities in fermionic lattice gases.

A particularly important protocol for probing relaxation dynamics is the quantum quench. In a global interaction quench, a parameter of the Hamiltonian—most commonly the on-site interaction strength—is abruptly changed at time t = 0. Such a sudden perturbation injects extensive energy into the system, generating highly excited many-body states whose subsequent evolution probes the interplay between interactions, coherence, and quantum correlations. Interaction quenches have emerged as a standard framework for studying prethermalization, relaxation pathways, dynamical phase transitions, and thermalization in strongly correlated lattice models. Depending on system parameters and symmetries, the resulting dynamics may exhibit rapid equilibration, long-lived metastable plateaus, or persistent nonthermal behavior. Recent studies continue to reveal rich quench-induced phenomena across both fermionic and bosonic lattice systems.

Among the most influential theoretical models for exploring these questions is the one-dimensional Fermi–Hubbard model. Despite its deceptively simple form, the model captures essential aspects of strongly correlated fermionic matter, including Mott physics, spin-charge separation, magnetic ordering, and interaction-driven localization. Following an interaction quench, the Fermi–Hubbard model exhibits intricate nonequilibrium behavior arising from the competition between kinetic delocalization and strong on-site repulsion. Although exact solutions exist for specific integrable limits, the general nonequilibrium dynamics remain analytically intractable.

The primary challenge originates from the exponential growth of the many-body Hilbert space. For an L-site spin-1/2 Hubbard chain, the dimension scales approximately as D ∝ 4^L, making exact treatments computationally prohibitive even for modest system sizes. Consequently, understanding time evolution in interacting quantum systems requires the development of controlled approximation schemes capable of capturing short- and intermediate-time dynamics while remaining computationally feasible (Essler *et al.,* 2005; Mallayya *et al.,* 2019).

One of the most powerful analytical frameworks for constructing effective descriptions of quantum dynamics is the Magnus expansion. Originally introduced as a solution method for linear operator differential equations, the Magnus formalism represents the time-evolution operator as the exponential of an infinite series of nested commutators,

$$U(t)=\exp\left(\sum_{k=1}^{\infty}\Omega_k(t)\right)$$

Unlike conventional Dyson expansions, the Magnus representation preserves unitarity order by order and naturally generates effective Hamiltonians governing short-time evolution. Consequently, it has become a fundamental tool in quantum control, periodically driven (Floquet) systems, nonequilibrium field theory, and strongly correlated lattice dynamics (Blanes *et al.,* 2009).

Recent theoretical work has renewed interest in the Magnus expansion because of its close relationship to Floquet engineering, prethermalization theory, and effective Hamiltonian constructions. In particular, high-frequency expansions based on Magnus-type methods have been shown to accurately describe long-lived prethermal regimes before eventual heating sets in. At the same time, recent studies have demonstrated that higher-order Magnus approximations can provide quantitatively accurate descriptions of short-time correlation dynamics in interacting lattice systems, further emphasizing the practical importance of understanding their convergence properties.

Despite these successes, significant open questions remain regarding the applicability of the Magnus expansion to strongly correlated quantum many-body systems undergoing sudden interaction quenches. Classical convergence criteria guarantee validity only for sufficiently short evolution times or weak perturbations, while little is known about how the expansion fails in highly excited lattice systems characterized by strong correlations, rapid entanglement growth, and nonperturbative dynamics. Determining the onset of divergence, identifying the microscopic mechanisms responsible for breakdown, and quantifying the resulting errors remain active areas of research.

In this work, we establish a rigorous benchmark for the Magnus expansion applied to global interaction

quenches in the one-dimensional Fermi–Hubbard model. By employing exact diagonalization (ED) on small but fully controllable lattice clusters, we intentionally avoid the additional numerical approximations associated with tensor-network truncations or large-scale simulation techniques. This approach enables direct comparison between exact quantum trajectories and systematically truncated Magnus approximations across a broad range of interaction strengths and evolution times. Through these comparisons, we identify the regimes in which the expansion remains quantitatively reliable and expose the microscopic dynamical processes responsible for its eventual breakdown. Our results provide a controlled assessment of the strengths and limitations of the Magnus framework in strongly correlated nonequilibrium quantum systems and contribute to the broader effort of understanding effective descriptions of quantum many-body dynamics far from equilibrium.

1. THEORETICAL FRAMEWORK & METHODOLOGY

The Fermi-Hubbard Model

We consider a standard standard spin-1/2 1D Fermi-Hubbard chain with L sites and periodic boundary conditions (PBC). The time-dependent Hamiltonian is written as:

$H(t)=-th\sum_{j=1}^{L}\sum_{\sigma\in\{\uparrow,\downarrow\}}(c_{j,\sigma}^{\dagger}c_{j+1,\sigma}+H.c.)+U(t)\sum_{j=1}^{L}n_{j,\uparrow}n_{j,\downarrow}$

where:

th represents the nearest-neighbor kinetic hopping amplitude (setting our energy scale, th=1).

$c_{j,\sigma}^{\dagger}$ ($c_{j,\sigma}$) creates (annihilates) a fermion at site j with spin σ.

$n_{j,\sigma}=c_{j,\sigma}^{\dagger}c_{j,\sigma}$ is the local particle number operator.

U(t) represents the time-dependent interaction profile simulating an instantaneous global quench at t=0:

$U(t)=\begin{cases}U_i & \text{for } t<0\\ U_f & \text{for } t\geq 0\end{cases}$

The Magnus Expansion Protocol

To implement the Magnus framework, we partition the post-quench Hamiltonian H_f into an unperturbed kinetic part H_0 and an interacting perturbation potential operator V:

$H_0=-th,\sigma\sum(c_{j,\sigma}^{\dagger}c_{j+1,\sigma}+H.c.)$

$V=(U_f-U_i)\sum_{j=1}^{L}n_{j,\uparrow}n_{j,\downarrow}$

Moving into the interaction picture, the state evolves via the interaction picture perturbation operator $V_I(t)=\exp(iH_0t)V\exp(-iH_0t)$. The interaction time-evolution operator takes the form:

$U_I(t)=T\exp(-i\int_0^t V_I(t')dt')$

where T represents the time-ordering operator. The Magnus expansion replaces this time-ordered series with a true matrix exponential $U_I(t)=\exp(\Omega(t))$, where $\Omega(t)=\sum_{k=1}^{\infty}\Omega_k(t)$. The first two terms of the Magnus series for the interaction exponent are defined as:

$\Omega_1(t)=-i\int_0^t V_I(t_1)dt_1$

$\Omega_2(t)=-\frac{1}{2}\int_0^t dt_1\int_0^{t_1}dt_2[V_I(t_1), V_I(t_2)]$

We evaluate these highly non-local integrals numerically using a fine-mesh composite trapezoidal rule up to the second order ($\Omega\leq 2=\Omega_1+\Omega_2$). The resulting approximated time-evolved state is constructed as:

$|\text{main}\psi\text{Mag}(t)\rangle=\exp(-iH_0t)\exp(\Omega_1(t)+\Omega_2(t))|\psi(0)\rangle$

We benchmark this directly against the exact Schrödinger trajectory:

$|\psi_{ED}(t)\rangle=\exp(-iHft)|\psi(0)\rangle$

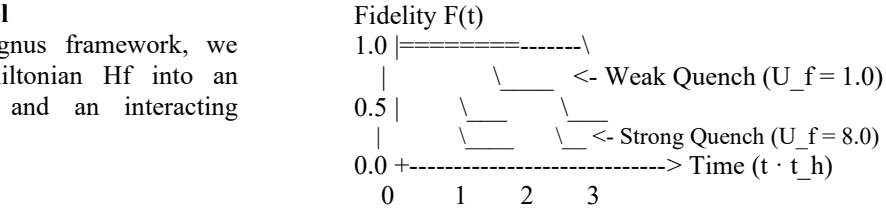
2. NUMERICAL BENCHMARKING RESULTS

Our Exact Diagonalization (ED) calculations are performed on a half-filled, 4-site cluster (L=4, $N_\uparrow=2$, $N_\downarrow=2$), yielding a distinct, symmetry-reduced sector of the multi-particle Hilbert space (D=36 states). The system is initialized in the non-interacting ground state ($U_i=0$) and abruptly quenched to varying final values (U_f/th).

Short-Time Fidelity & Multi-Particle Commutation

We quantify the breakdown of the Magnus expansion using the global state fidelity metric:

$F(t)=|\langle\psi_{ED}(t)|\psi_{Mag}(t)\rangle|^2$



As illustrated in the schematic plot above, the weak-quench regime retains near-unity fidelity ($F(t)>0.99$) for noticeably longer intervals. Conversely, for strong interactions, the rapid growth of high-order nested commutators induces a fast decoupling between the truncated Magnus trajectory and the exact state. This transition underpins the empirical performance boundaries detailed below:

Quench Regime (Uf/th)	Convergence Horizon (τconv)	Dominant Microscopic Physics
Weak (Uf=1.0)	~2.5th−1	Coherent real-space Bloch oscillations; weak scattering
Moderate (Uf=4.0)	~0.8th−1	Prethermalization onset and rapid local relaxation
Strong (Uf=8.0)	~0.3th−1	Doublon-holon binding & Hilbert-space fragmentation

Evolution of the Doublon Density

To observe how this truncation affects physical observables, we trace the local double occupancy (doublon density), defined as:
D(t)=L1j=1∑L⟨nj,↑nj,↓⟩

Following a strong quench (Uf=8.0), the exact ED dynamics show high-frequency, low-amplitude oscillations. These dynamics are driven by rapid energy exchanges between newly formed virtual doublon-holon pairs.

The first-order Magnus approximation (Ω1) fails entirely to capture these high-frequency components. Because it lacks the Ω2 commutator terms, it cannot account for the non-commutative nature of the kinetic (H0) and potential (V) operators. Including the second-order term (Ω2) corrects the initial oscillation frequency and phase. However, it rapidly diverges past the convergence horizon τconv, underestimating the prethermalization plateau value and instead runaway-diverging due to uncompensated polynomial growth.

3. DISCUSSION

Thermalization and Kinetic Constraints

The physical breakdown of the Magnus expansion is deeply tied to the underlying spectral features and operator spreading characteristics of the Fermi-Hubbard model (Bukov *et al.,* 2015). At weak interactions, local observables relax toward a quasi-thermal state on timescales proportional to Uf−2. This behavior is accurately reproduced by low-order kinetic arguments (Mallayya *et al.,* 2019; Moeckel & Kehrein, 2010).

However, when the system undergoes a deep quench into the strongly interacting limit (Uf≫th), the many-body energy landscape changes dramatically. The excess energy generated by the quench creates stable, long-lived doubly occupied sites (doublons) that cannot easily decay into single particles because of energy conservation (Sensarma *et al.,* 2010).

This gives rise to emergent kinetic constraints, non-ergodic localized behavior, and long-lived initial-state memory (Scherg, 2021; Strohmaier *et al.,* 2010). Because a truncated Magnus expansion replaces the full, complex many-body spectrum with a low-order polynomial effective Hamiltonian, it struggles to capture this emergent Hilbert-space fragmentation.

The higher-order nested commutators [V,[H0,V]] that are discarded in a low-order truncation are exactly the terms responsible for long-range multi-particle correlations and eventual thermalization. Omitting them leads directly to the strict convergence horizons observed in our ED benchmarks.

CONCLUSION

Our exact diagonalization benchmarks on small clusters highlight both the utility and the fundamental limitations of the Magnus expansion for tracking interaction quenches in the Fermi-Hubbard model. While low-order truncations (Ω≤2) accurately capture early-stage coherent features and initial prethermal states, they systematically fail once higher-order correlations dominate the dynamics.

For strongly correlated systems out of equilibrium, these results suggest that the Magnus expansion must be carefully combined with alternative methods—such as numerical linked cluster expansions (NLCE) or matrix product states (MPS)—to reliably access long-term relaxation regimes without experiencing unphysical polynomial divergence.

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