Optimal control for unitary preparation of many-body states: application to Luttinger liquids

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Many-body ground states can be prepared via unitary evolution in cold atomic systems. Given the initial state and a fixed time for the evolution, how close can we get to a desired ground state if we can tune the Hamiltonian in time? Here we study this optimal control problem focusing on Luttinger liquids with tunable interactions. We show that the optimal protocol can be obtained by simulated annealing. We find that the optimal interaction strength of the Luttinger liquid can have a nonmonotonic time dependence. Moreover, the system exhibits a marked transition when the ratio $\tau/L$ of the preparation time to the system size exceeds a critical value. In this regime, the optimal protocols can prepare the states with almost perfect accuracy. The optimal protocols are robust against dynamical noise.

Loading cold atomic gases into optical lattices provides an opportunity to study the nonequilibrium properties of quantum matter in thermally isolated and highly tunable environments [1, 2]. The central object of such studies is a many-body quantum state which undergoes unitary evolution generated by a time-dependent local Hamiltonian.

In an important class of problems, we are interested in using the unitary evolution to transform an initial state that is the ground state of a local Hamiltonian to the ground state of another Hamiltonian. Such problems are relevant for the preparation of states in regimes where direct equilibration is difficult [3–5]. Ground states preparation is the key to simulating many-body Hamiltonians, such as the Hubbard model, which can be realized with cold atoms [6, 7].

If one had infinite time to wait, according to the adiabatic theorem of quantum mechanics, the unitary transformation can be done with arbitrary accuracy in any finite system. Extrinsic losses and quantum decoherence, however, set an upper bound on the practical time to carry out the process. In any finite time $\tau$, nonadiabatic effects are unavoidable [8]. These effects are most severe in the absence of an energy gap [9]. In this paper we focus precisely on dynamics within the gapless phase by studying Luttinger liquids.

Let us start by casting the question of finding the optimal dynamical protocol in a generic way. Assume we have a local Hamiltonian $H(\{g\}) = \sum_{i=1}^{M} g_{i} O_{i}$ where the $O_{i}$s are local operators and the $g_{i}$s are coupling constants that, within a given range, can be tuned to any value as a function of time. We would like to transform $|\Psi_{1}\rangle$ which is the ground state of $H(\{g_{1}\})$ to $|\Psi_{2}\rangle$, the ground state of $H(\{g_{2}\})$ in a given time $\tau$. How close can the final state $|\Psi(\tau)\rangle = T \exp[-i \int_{0}^{\tau} dt' H(\{g(t')\})] |\Psi_{1}\rangle$ be to the desired ground state $|\Psi_{2}\rangle$? Here $T$ represents time-ordering.

The meaning of closeness above depends on the measure used. There are several popular measures like the excess energy for example [10]. Here we use the wave function overlap

$$F(\{g(t)\}) = \langle \Psi(\tau) | \Psi_{2}\rangle^2. \quad (1)$$

The problem is then reduced to finding the time-dependent $\{g(t)\}$ that maximizes the functional above. This interesting question in quantum dynamics [8] is in fact a typical problem in optimal control theory as noted in Ref. [11, 12]. Let us emphasize that we are concerned only with the final state and maintaining adiabaticity during the evolution, as for example in Ref. [13], is not a constraint. Moreover, we are restricted to local Hamiltonians allowed by the experimental setup.

The focus of this work is the Luttinger model for interacting fermions in one space dimension, whose Hamiltonian can be written in momentum space as follows

$$H = u \sum_{q > 0} \left( K \Pi_{q} \Pi_{-q} + \frac{1}{K} q^{2} \Phi_{q} \Phi_{-q} \right) \quad (2)$$

where $\Phi_{q}$ are bosonic fields and $\Pi_{q}$ their conjugate momenta. The parameters $u$ and $K$ are respectively the velocity of the charge carriers and the Luttinger parameter. We consider a fixed number of particles, focusing on the half-filled case. The zero mode, which is responsible for changing the particle number sector in the bosonized description, is therefore excluded in the above expression. Assuming we have an odd number of sites $L$ in the system, the momenta $q$ are given by $q = 2\pi n/L$ for $n = 1, \cdots, L/2$.

This Luttinger Hamiltonian is the low-energy effective theory for models of interacting fermions on a one-dimensional lattice, in particular the 1D Hubbard model

$$H = \sum_{j} \left[ -c_{j}^{\dagger} c_{j+1} + \text{h.c.} + V(n_{j} - \frac{1}{2})(n_{j+1} - \frac{1}{2}) \right]. \quad (3)$$

Since spin degrees of freedom are not essential for our discussion, here we focus on spinless fermions. With the hopping amplitude set to unity as in Eq. (3), the Luttinger parameters $u$ and $K$ are related to $V$ via the Bethe ansatz (see Ref. [14] for example).

We will consider trajectories for $u$ and $K$ that are parametrized by a time-dependent $V(t)$: $u = u(V)$ and $K = K(V)$. The strength of Hubbard-type interactions can be tuned in optical lattices both by manipulating the optical potential with lasers [15–17] and through Feshbach resonances controlled with magnetic fields [17, 18].

Notice that while the relation between the Luttinger liquid (LL) and the 1D Hubbard model holds at low energies, the results we find for the optimum dynamical protocol in the former should be applicable to the latter when the total momentum $qn_{q}$ in each harmonic oscillator mode in Eq. (2), where
of the global minimum. In this regime, finding the global minimum becomes exceedingly difficult, particularly for larger systems. Nevertheless, we can tackle this problem using a two-stage approach. For smaller systems, we can directly compute the overlap against the ground state using unbiased Monte Carlo (MC) simulations. For larger systems, we can use approximate methods based on the Sorensen-Schuster protocol [22].

Maximizing the overlap with the ground state for a single critical point can be viewed as a two-stage process. In the first stage, we find the optimal protocol by maximizing the overlap against the ground state, and in the second stage, we improve the overlap by using the optimal protocol.

We consider the problem of transforming the system initially at the ground state into a target state that is far from the ground state. This is tantamount to maximizing the function

\[
\mathcal{F}(V_{1}, \ldots, V_{N}) = \exp \left( \sum_{q > 0} \ln \left( 4 \alpha_{2} \frac{\Re z_{q}(\tau)}{|\alpha_{2} + z_{q}(\tau)|^{2}} \right) \right).
\]

The overlap above is written as a multi-variable function of \(V_{j}\). To find the optimal protocol, we minimize the cost function \(E(\{V_{j}\}) = -\ln \mathcal{F}(\{V_{j}\})\) with respect to the configuration \(\{V_{j}\}\). This can be done by Monte-Carlo (MC) methods. We perform simulated annealing calculations with kinetic moves consisting of random small changes in randomly chosen \(V_{j}\).

We compare the results of the optimal protocol against two additional calculations. We consider the one-parameter variational protocol \(V(t) = V_{1} + (V_{2} - V_{1})(t/\tau)\) and calculate the final overlap for the linear \((r = 1)\) as well as for the best power-law protocols \((r = r_{\text{min}} = 0)\). The optimal protocol found by MC simulations performs significantly better than both of the above.

In Fig. 1, we show the final \(E\) for the optimal protocol obtained by an unbiased MC simulation as well as for the linear and the best power-law protocols for \(V_{2} = -1.5\) and several system sizes. When \(\tau/L\) becomes larger than a critical value, the final \(E\) obtained by MC optimization exhibits a qualitative change of behavior and shoots down by several orders of magnitude.

The value of the cost function obtained by MC simulations is generically only an upper bound on the actual minimum. For \(\tau < \tau_{c} \propto L\), different annealing histories lead to a unique protocol suggesting that the the minimum found is likely the global minimum. For \(\tau > \tau_{c}\) however, we never converge to a unique protocol indicating that we have only found a local minimum. In this regime, finding the global minimum becomes exceedingly difficult, particularly for larger systems due to the increased computational complexity. Nevertheless, notice that the minima we find have \(\mathcal{E}(\tau)\) very close to zero and can prepare the new ground state almost exactly.

Although it is not clear from the finite-size scaling of the obtained \(\mathcal{E}(\tau)\) that there is a transition in the thermodynamic limit, the drastic change of the system behavior strongly suggests the presence of a true transition for the global minimum.
FIG. 1. The final $E$ obtained by Monte-Carlo (MC) simulations compared with the linear and best power-law protocols. The final $E$ plunges by several orders of magnitude for $\tau/L > \tau_c/L \approx \frac{1}{8}$ (marked with a star). Note that in this regime, the data merely represents an upper bound on $E(\tau)$ and the actual cost function could be even smaller.

Note that the local minima we find are expected to be closer to the actual global minimum for smaller systems.

An interesting feature of the optimal protocols is that, as seen in Fig. 2, the interaction strength can be an oscillatory function of time. Note that increasing the number of discretization points $N$.

For the many-mode problem, we wish to have $z_q(\tau) = \alpha_2$ for all the modes. From the discussion of the single-mode case above, we find that, for times larger than some $\tau \propto L$, an infinite number of solutions exists for the slowest mode ($q = \frac{2\pi}{L}$) and consequently for every individual mode $q$. Since the system of equations $z_q(\tau) = \alpha_2$, $\forall q$ is under-determined when the number of variational parameters is larger than $L - 1$, it seems plausible that for $\tau > \tau_c \propto L$, one can simultaneously satisfy $z_q(\tau) = \alpha_2$ for all modes. We have not, however, been able to explicitly find such exact solutions for the many-mode problem and thus cannot rule out the possibility that the transition at $\tau > \tau_c \propto L$ happens because $|z_q(\tau) - \alpha_2|$ for all modes can become infinitesimally small rather than exactly zero.

Before proceeding, let us check the applicability of the results obtained for the Luttinger model Eq. (2) to the Hubbard model Eq. (3). We need to calculate the total mode momentum $qn_q$. Writing the occupation number as $n_q = \langle \varepsilon_q \rangle / 2\varepsilon_0 - 1/2$ where $\varepsilon_0$ is the ground-state energy of a mode, we obtain

$$n_q(t) = \frac{1}{2\pi\tau_c(t)} \left( K(t) |z_q(t)|^2 + \frac{1}{K(t)} \right) - \frac{1}{2}.$$  

We find that when the final overlap is large, the evolution does not typically excite electrons too far away from the Fermi surface. For example, the protocol for $L = 129$ and $\tau = 16$ in Fig. 2 has $\max_{q,t} |qn_q(t)| = 0.302$ which is indeed in the linear regime.

From the experimental point of view, the extremely small $E(\tau)$ obtained in the regime $\tau > \tau_c$ can be very useful for the preparation of many-body states. In practice however, there are always inaccuracies in the experimental implementation of a prescribed protocol. We check the robustness of these protocols against random perturbations $\delta V(t)$ taken from a uniform distribution $[-W/2 \ldots W/2]$ for each segment of the
FIG. 4. Left: the noise-averaged $\overline{E(\tau)}$ as a function of $W$ for a random noise $\delta V(t)$ taken from a uniform distribution $[-W/2, \ldots, W/2]$. Right: final cost $\overline{E(\tau)}$ as a function of $V_1$ where the initial wave function is the ground state for interaction strength $V_1 - \delta V_1$. The plots are for $L = 65$, $\tau = 16$ and $V_2 = -1.5$.

piece-wise constant $V(t)$. We also check the effect of errors in the initial wave function by applying the protocol to the ground state for $V_1 - \delta V_1$ instead of $V_1$.

In Fig. 4, we show $\overline{E(\tau)}$ as a function of $\delta V_1$ in addition to the noise-averaged $\overline{E(\tau)}$ as a function of $W$ for the MC optimized, best power-law and linear protocols and for $L = 65$, $\tau = 16$ and $V_2 = -1.5$. As seen in the figure, even for large noise of the order a few percent of the bandwidth, the MC optimized protocols yield much smaller $\overline{E(\tau)}$ than the power-law and linear $V(t)$. These studies indicate that, practically, using the optimal protocols is advantageous even in the presence of experimental errors and inaccuracies.

To better understand the effects of this dynamical noise on the behavior of thermally isolated Luttinger liquids, we consider a simple case. We assume we are initially in the ground state for interaction strength $V_0$ (with corresponding $u_0$ and $v_0$) and $V(t) = V_0 + \delta V(t)$ for a time $\tau$ where $\delta V(t)$ is a random noise of strength $W$. For $W = 0$, the wave function remains in the ground state and $\overline{E(\tau)} = 0$. For small $W$, we can linearize Eq. (6) and write $i \delta z_{q}(\tau) = 2i q u_0 \delta \alpha(t) \frac{1}{2}\int dt e^{i 2 q u_0 (t - \tau)} \delta \alpha(t)$. (9)

Using Eq. (1), we get $\overline{E(\tau)} = \frac{1}{2\pi^2} \sum_{q > 0} |\delta z_{q}(\tau)|^2 + \mathcal{O}(\delta z_0^3)$ which assuming uncorrelated noise $\langle \delta \alpha(t) \delta \alpha(t') \rangle$ is $W^2 \delta(t-t')$ and using Eq. (9) above leads to $\overline{E(\tau)} \propto W^2$. Note that since $\tau_c \propto L$, strong noise limits the size of the systems which can be accurately prepared. Also notice that $|\delta z_{q}(\tau)|^2 \approx q^2$ and in contrast to coupling to a thermal bath, the dynamical noise discussed above creates more excitations in modes with higher momentum. The effect of noise on a time-dependent optimal protocol seen in Fig. 4 is mathematically more complicated but essentially similar to this simple case. The noise-averaged $\overline{E(\tau)}$ grows as a power law with $W$ with an exponent that depends on $V_1$ and $V_2$.

In summary, we used simulated annealing to address an outstanding problem in the nonequilibrium dynamics of interacting quantum systems, namely finding unbiased optimal protocols for unitary preparation of strongly correlated states. We focused on transforming states in the LL phase of interacting fermions with tunable interaction strength. Unbiased optimization over all ramp shapes yields nonmonotonic optimal protocols. The behavior of the system exhibits a marked transition for $\tau > \tau_c \propto L$ where the states can be transformed with almost perfect accuracy. The optimal protocols are robust against noise, which makes them of practical experimental importance for the preparation of states in cold atomic systems.

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Supplemental Material for “Optimal control for unitary preparation of many-body states: application to Luttinger liquids”

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Abstract

The trajectories of \( z_q(t) \) on the complex \( z \) plane are discussed for the evolution with optimal protocols.

Some intuition may be gained regarding the appearance of oscillations in optimal protocols discussed in the main text by considering the trajectories of \( z_q(t) \) on the complex \( z \) plane. The evolution of the system is governed by a set of nonlinear differential equations (Eq. (6) of the main text) for many modes. We would like controls \( \alpha(t) \) and \( u(t) \) such that for all modes \( q \), the complex function \( z_q(t) \) moves from the initial value \( z_q(0) = \alpha_1 \) to a desired final value \( \alpha_2 \) in a time \( \tau \). Now the quantity controlling this evolution for each mode is \( q\tau \) as discussed in the main text. It is evident from Eq. (6) of the main text that \( z_q \) moves faster for modes with higher momenta. To get to the same point \( \alpha_2 \), we find that \( z_q \) actually winds around in the complex plane as seen in Fig. 1. The appearance of these windings, i.e. oscillations in the imaginary part of \( z_q \), is rather intuitive. One may guess that an oscillatory control is required to generate the winding of the complex \( z_q(t) \).

Figure 1: The values of \( z_q(t) \) for three different modes during the evolution with the MC optimized protocol with \( L = 65, \tau = 16 \) and \( V_2 = -1.5 \). As the momentum \( q \) increases the modes wind around in the complex plane to reach the point \( \alpha_2 \).