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

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Many-body ground states of local Hamiltonians 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 using the simulated annealing method. Rather surprisingly, we find that in the Luttinger liquid case the interaction strength in the optimal protocol can have a *non-monotonic* time-dependence. We find a marked difference in the behavior of the system when the ratio τ/L of the preparation time to the system size exceeds a critical value around 1/8. In this regime, the optimal protocol can prepare the states with almost perfect accuracy. Finally, we argue that the time-scale of the optimal evolution defines a dynamical measure of distance between quantum states.

The ability to manipulate systems of atomic gases loaded onto optical lattices, together with the fact that these systems are quite well isolated from their environment, provides an opportunity to explore the non-equilibrium properties of quantum matter [1, 2]. The central object in such studies is a many-body quantum pure state undergoing unitary evolution generated by a time-dependent local Hamiltonian.

Unitary evolution is of course not confined to the ground state manifold. In an important class of problems, however, we are specifically interested in transforming an initial state that is the ground state of a local Hamiltonian to the ground state of another Hamiltonian via the unitary evolution. Such problems appear for example in the context of the adiabatic quantum computing [3] or for the preparation of non-trivial ground states in regimes where direct cooling is difficult [4–6]. Ground state preparation is the key to simulating many-body model Hamiltonians with cold atoms.

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 τ non-adiabatic effects are therefore unavoidable [7]. These effects are most severe in the absence of an energy gap [8]. In this paper we focus precisely on dynamics within the gapless phase by studying unitary evolution in the Luttinger liquid.

Let us start by casting the question of finding the optimal dynamical protocol in a generic way. Assume we have a local Hamiltonian with a finite number of terms

$$H(\{g\}) = \sum_{i=1}^{M} g_i \, O_i$$

where the O_is are local operators and the g_is 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 τ. Assuming we are able to give *any* time-dependence to the coupling constants $\{g\}$, how *close* can the final state

$$|\Psi(\tau)\rangle = \mathcal{T} e^{-i\int_0^\tau dt' H(\{g(t')\})} |\Psi_1\rangle$$

be to the desired ground state $|\Psi_2\rangle$? Here $\mathcal{T}$ represents time-ordering. The precise meaning of *closeness* above depends on the measure used. There are several popular measures like the excess energy or the density of quasi-particle excitations. Here we use the wave function overlap

$$\mathcal{F}[\{g(t)\}] = |\langle\Psi(\tau)|\Psi_2\rangle|^2. \tag{1}$$

The final overlap depends upon the ramp shape $\{g(t)\}$ [11] and the problem is then reduced to finding the time-dependent $\{g(t)\}$ that maximizes the functional above. This interesting open question in quantum dynamics [7] is in fact a typical problem in optimal control theory, a field of applied mathematics with a wide range of applications from engineering to social science. Let us emphasize that in this optimal control problem, we are concerned only with the *final* state and maintaining *adiabaticity* during the evolution, as for example in Ref. [9], is *not* a constraint.

The focus of this work is the Luttinger model, whose Hamiltonian density is given by the following quadratic form

$$\mathcal{H} = \frac{u}{2}\left(K\,\Pi^2(x) + \frac{1}{K}(\nabla\Phi(x))^2\right)$$

where $\Phi(x)$ is a bosonic field related to the charge density via $\rho(x) = \nabla\Phi(x)/\sqrt{\pi}$ and $\Pi(x)$ is its conjugate momentum. The parameters u and K are respectively the velocity of the charge carriers and the Luttinger parameter. In Fourier space, we can then write the Hamiltonian as follows

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

where Φ_q are bosonic fields and Π_q their conjugate momenta with $[\,\Phi_q, \Pi_{q'}\,] = i\delta_{qq'}$. We consider the problem where particle number is fixed, focusing explicitly the case of half-filling, and therefore we have excluded in the above expression the zero mode which is responsible for changing the particle number sector in the bosonized description. Assuming

we have an odd number of sites L in the system, the momenta q are given by $q = 2\pi \frac{n}{L}$ for $n = 1 \cdots, \frac{L-1}{2}$.

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

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

With the hopping amplitude t set to unity, the Luttinger parameters u and K are related to V via the Bethe ansatz (see Ref. [13] for example). We will consider trajectories for u and K that are parametrized by a time-dependent $V(t)$: $u = u(V)$ and $K = K(V)$. 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 later when the total momentum qn_q in each harmonic oscillator mode in Eq. (2), where n_q is the occupation number, is small compared to $\pi/2$. (We will indeed check a posteriori that for all optimal protocols that yield high final overlaps, this condition is satisfied at all times during the evolution.)

At half filling, the gapless Luttinger liquid (LL) description holds for $-2 < V/t < 2$. At $V/t = 2$, the system becomes unstable to charge density wave (CDW) order and a gap opens up. An optimal power-law protocol for bringing the system from the gapped phase to the critical point was found in Ref. [10] using adiabatic perturbation theory [12]. Here we consider the problem of transforming the system initially at the CDW phase transition critical point to a point deep within the gapless LL phase.

We proceed by expressing $\Pi_q = -i\, \partial_{\Phi_q}$. The many-body ground state wave function (in the $|\{\Phi_q\}\rangle$ basis) is

$$\Psi(\{\Phi_q\}) = \prod_{q>0} [\, \psi_q(\phi_q, K)\, \psi_q(\varphi_q, K)\,] \tag{4}$$

where ϕ_q and φ_q are respectively the real and imaginary parts of Φ_q and

$$\psi_q(\phi, K) = \left(\frac{2\,q}{\pi K}\right)^{\frac{1}{4}} \exp\left(-\frac{q}{K}\phi^2\right).$$

Let us assume we are initially in the ground state for $K_1 = K(V_1)$ (at the phase transition point $V = 2$, $K = \frac{1}{2}$). We would like to find the time-dependent interaction strength $-2 < V(t) < 2$ for t between 0 and τ that yields the maximum overlap with the ground state corresponding to V_2 at time τ.

At intermediate times, the wave function remains a product $\prod_{q>0} [\Psi_q(\phi_q, t)\Psi_q(\varphi_q, t)]$ where $\Psi_q(\phi, t)$ is the solution of the following Schrödinger equation:

$$\left[i\partial_t - u(t) \left(-\frac{K(t)}{4}\, \partial_\phi^2 + \frac{1}{K(t)}\, q^2\, \phi^2 \right) \right] \Psi_q(\phi, t) = 0$$

with the initial condition $\Psi_q(\phi, 0) = \psi_q(\phi, K_1)$. Up to an unimportant overall phase, the solution of the above differential equation is

$$\Psi_q(\phi, t) = \left(\frac{2\,q}{\pi}\right)^{\frac{1}{4}} [\Re\, z_q(t)]^{\frac{1}{4}} \exp\left(-q\, z_q(t)\, \phi^2\right) \tag{5}$$

where $\Re$ indicates the real part and $z_q(t)$ is a complex-valued function that satisfies the following Riccati equation:

$$i\, \dot{z}_q(t) = q\, \frac{u(t)}{\alpha(t)}\, \left[z_q^2(t) - \alpha^2(t) \right] \tag{6}$$

with $\alpha(t) \equiv 1/K(t)$ and the initial condition $z_q(0) = \frac{1}{K_1}$.

To perform the optimization for the many-body system, we discretize time and approximate a general $V(t)$ by a piecewise constant function over the interval $[0 \ldots \tau]$. This allows us to write the final overlap, which is a functional of $V(t)$, as a multi-variable function that can be maximized numerically. An optimal protocol is found once there is convergence in the final overlap as we increase the number of discretization points.

Physically, the piecewise-constant function describes a sequence of sudden quenches. Let us assume a sequence V_j with $j = 1 \ldots N$ such that $V(t) = V_j$ for $(j-1)\Delta t < t < j\Delta t$ with $\Delta t = \tau/N$. We then get two corresponding sequences u_j and α_j. If $z_q^j \equiv z_q(j\Delta t)$, we obtain the following recursion relation for z_q^j by solving Eq. (6) for time-independent u and α,

$$z_q^j = i\, \alpha_j\, \tan\left[q\, u_j\, \Delta t + \arctan\left(-i \frac{z_q^{j-1}}{\alpha_j} \right) \right]. \tag{7}$$

Our focus here is finding an optimal protocol but Eq. (7) above is of interest in its own right since it gives an exact solution of the non-equilibrium wave-function for any sequence of sudden quenches in the interaction strength. Notice that once we know $z_q(t)$ for all modes, we have the many-body wave-function as a simple product of single mode wave-functions.

Recursively solving the above relation Eq. (7) yields $z_q(\tau) = z_q^N$ for any given piece-wise constant interaction strength. The overlap Eq. (8) can then be determined from $z_q(\tau)$ as follows

$$\mathcal{F}(V_1, \ldots V_N) = \exp\left[\sum_{q>0} \ln\left(4\, \alpha_2\, \frac{\Re\, z_q(\tau)}{|\, \alpha_2 + z_q(\tau)\, |^2} \right) \right]. \tag{8}$$

where $\alpha_2 \equiv 1/K_2$.

The overlap above is written as a multi-variable function of $\{V_j\}$. To find the optimal protocol, we minimize the cost function $\mathcal{E}(\{V_j\}) \equiv -\ln \mathcal{F}(\{V_j\})$ with respect to the configuration $\{V_j\}$. Many methods for finding the minimum of a function of multiple variables, such as the conjugate gradiants, are geared toward finding a local minimum and are not suitable for our problem due to the presence of many such minima. Monte-Carlo methods on the other hand have a better chance of finding the global minimum. We do simulated

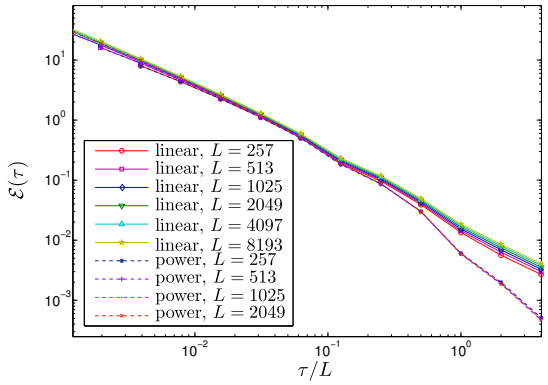

FIG. 1. The final $\mathcal{E}$ vs. τ/L for the linear and the best power-law protocols and several system sizes.

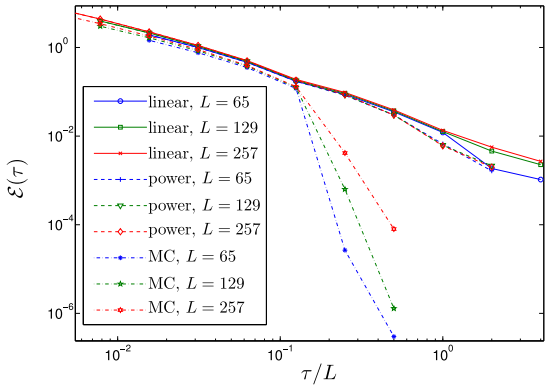

FIG. 2. The final $\mathcal{E}$ obtained by Monte-Carlo (MC) simulations compared to the linear and best-power-law protocols. The final $\mathcal{E}$ plunges by several orders of magnitude for τ/L approximately larger than $\frac{1}{\infty}$. Note that in this regime, the data merely represents an upper bound on $\mathcal{E}(\tau)$ and the actual overlap could be even better. This upper bound already provides almost perfect overlap.

annealing calculations with kinetic moves consisting of a random small change in a randomly chosen V_j.

We compare the results of the optimal protocol against two additional calculations. We consider the one-parameter variational protocol $V(t) = V_1 + (V_2 - V_1)\,(t/\tau)^r$ for $0 < t < \tau$ and calculate the final overlap for the linear protocol ($r = 1$) as well as for the the best power-law protocol ($r = r_{\min}$ with $\partial_r\, \mathcal{E}(r) = 0$). The optimal protocol found by Monte-Carlo simulations performs significantly better than both of the above.

The final $\mathcal{E}(\tau)$ is plotted in Fig. 1 as a function of τ/L for the linear and the best-power-law protocols and for several system sizes. It appears from the collapse of the data that for the best-power-law protocol, the final $\mathcal{E}$ is a function of τ/L only. The linear protocol however exhibits corrections to scaling of the form $\mathcal{E}(\tau, L) = f(\tau/L) \ln L$. This suggests that in the thermodynamic limit, the linear protocol leads to orthogonal wave functions for any finite τ/L. The optimal exponent $r_{\min}(\tau, L)$ has a cross-over from a function of τ only for short times to a function of τ/L for longer times.

In Fig. 2, we show the final $\mathcal{E}$ for $L = 65$, 129 and 257 for the optimal protocol obtained by an unbiased Monte-Carlo simulation. We also plot $\mathcal{E}$ for the linear and best power-law protocols for comparison. When τ/L becomes larger than a critical value, the final $\mathcal{E}$ obtained by Monte-Carlo optimization exhibits a qualitative change of behavior and shoots down by *several* orders of magnitude. Using the protocol obtained by Monte-Carlo, we can then prepare the quantum states with virtually *perfect* accuracy as long as $\tau > \tau_c \propto L$. In this regime, the convergence is not very good and the value of the cost function obtained by Monte-Carlo simulations is merely an upper bound on the actual minimum. For shorter times on the other hand, we have good convergence as the number of discretization points N is increased.

Notice that despite the qualitative change of behavior, it is not clear from the finite-size scaling of the obtained $\mathcal{E}(\tau)$ that there is a transition in the thermodynamic limit. Nevertheless, we observe that the difficulty in convergence becomes more severe for larger systems. This implies that the upper bound found by Monte-Carlo simulations becomes looser as the system size is increased. We also observe that different initial conditions and annealing histories lead to different protocols with close cost $\mathcal{E}(\tau)$ in the $\tau > \tau_c$ regime. The difficulty of convergence to a unique optimal protocol in this regime is reminiscent of the complex energy landscape in glasses. In this case finding the global minimum becomes exceedingly difficult, specially for larger systems, due to the presence of many local minima.

We can speculate a possible explanation for this behavior. Naively, we expect to be able to find an exact solution $\mathcal{E}(\tau) = 0$ if we have $N = L - 1$ unknowns $\{V_j\}$ to solve the $L - 1$ equations $z_q(\tau) = \alpha_2$ for all modes. This is of course not possible for short τ even if $N \gg L$. When the time τ become of order L, the equation $z_q(\tau) = \alpha_2$ becomes consistent under-determined for any single mode q for large N. Simultaneously solving the equations above for all modes is a much more complex problem however and an exact solution may need longer times than $\tau = \mathcal{O}(L)$ (possibly exponential). Nevertheless, the complexity of the energy landscape may be related to having consistent under-determined equations that, for each mode q, admit an infinite number of solutions to the inequality $|z_q(\tau) - \alpha_2| < \epsilon$ with an infinitesimal ϵ. In this case, a large number of such solutions may simultaneously satisfy the inequality for all modes.

A striking feature of the optimal protocol as seen in the Fig. 3 is that the interaction strength is a monotonic oscillatory function. Fig. 3 shows the convergence of the optimal protocol with increasing the number of discretization points. For large enough systems, the period of the oscillation does not have a strong dependence on the system size L or the preparation time τ. The oscillations therefore are a consequence of short-distance physics, i.e. the discrete lattice. The short distance length scale is the lattice spacing which is set to one

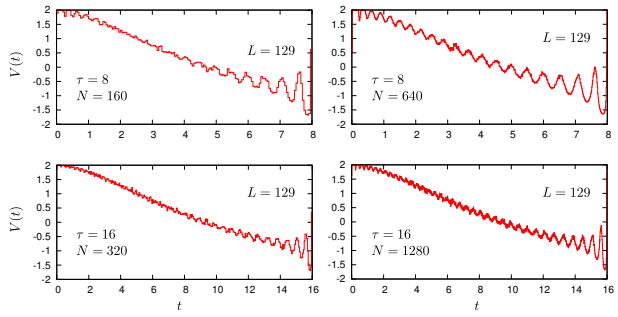

FIG. 3. The interaction strength $V(t)$ as a function of time for the optimal protocol obtained by Monte-Carlo simulations. With increasing the number of discretization points N, the optimal protocol converges to a non-monotonic oscillatory function.

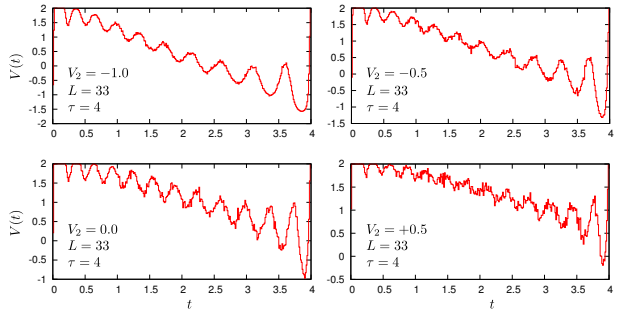

FIG. 4. The optimal protocol interaction strength $V(t)$ for different values of V_2.

in our problem. As seen Fig. 4, the period of the oscillations decreases as V_2 becomes larger. This observation is consistent with a short-distance cut-off controlling the oscillations since the velocity $u(V)$ is an increasing function of the interaction strength V.

To check the applicability of the results to the Hubbard model, we consider the occupation number of modes n_q. Writing the occupation number as $n_q = \langle \varepsilon_q \rangle / 2\varepsilon_q^0 - 1/2$ where ε_q^0 is the ground state energy of a mode, we obtain

$$n_q(t) = \frac{1}{4\Re z_q(t)} \left(K(t) \left| z_q(t) \right|^2 + \frac{1}{K(t)} \right) - \frac{1}{2}. \quad (9)$$

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. 3 has $\max_{q,t} [q n_q(t)] = 0.302$ which is in the linear regime.

We now discuss a new measure of distance between quantum states based on optimal preparation. The dual problem to finding an optimal protocol for a given time τ is finding the minimum time required to reach a given wave function overlap, namely $\tau_{\min}(L, \mathcal{E})$. In the asymptotic limit of $L \to \infty$ and $\mathcal{E} \to 0$, we expect $\tau_{\min} \sim f(L) g(\mathcal{E})$. The $\mathcal{E}$ found in Fig. 2 for example has different asymptotic forms $g(\mathcal{E})$ but the same $f(L) \sim 1/L$ for both the optimal and best-power-law protocols. The asymptotic form for $\tau_{\min}$ defines a dynamical measure of distance between the ground states $|\Psi_1\rangle$ and $|\Psi_2\rangle$. This new measure of distance can lead to a new classification of quantum phases relevant for non-equilibrium physics. The importance of local unitary transformations, such as the ones generated by the Hamiltonian evolution, in classifying states was recently pointed out in [15].

In summary, we used simulated annealing to address an outstanding open problem in the non-equilibrium dynamics of interacting quantum systems, namely finding unbiased optimal protocols for unitary preparation of strongly correlated states. We focused on transforming states in the Luttinger liquid phase of interacting fermions with tunable interaction strength. Quite surprisingly, we found optimal protocols that exhibit oscillatory behavior. For τ/L larger than a critical value, we found that the states can be transformed with almost perfect accuracy. Finally, based on this optimal control problem, we defined a new measure of distance between quantum ground states that is relevant for out-of-equilibrium physics.

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