Time-dependent variational principle in matrix-product state manifolds: pitfalls and potential

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We study the applicability of the time-dependent variational principle in matrix product state manifolds for the long time description of quantum interacting systems. By studying integrable and nonintegrable systems for which the long time dynamics are known we demonstrate that convergence of long time observables is subtle and needs to be examined carefully. Remarkably, for the disordered nonintegrable system we consider the long time dynamics are in good agreement with the rigorously obtained short time behavior and with previous obtained numerically exact results, suggesting that at least in this case the apparent convergence of this approach is reliable. Our study indicates that while great care must be exercised in establishing the convergence of the method, it may still be asymptotically accurate for a class of disordered nonintegrable quantum systems.

Introduction.— The numerically exact simulation of the dynamics of strongly interacting quantum systems is a grand challenge in condensed matter science. For ground states of gapped one-dimensional systems with short-range interactions, the density matrix renormalization group (DMRG) proves to be a powerful and efficient approach [1, 2]. Its success is linked to the fact that the ground states of these systems are optimally representable by matrix product states (MPS), with a moderate number of variational parameters, normally referred to as the bond dimension. While DMRG has been extended into the time-domain, the timescales that may be reached are usually quite short as a consequence of correlations that develop within the propagated wavefunction [1, 2]. Time evolution tends to quickly displace states from the space efficiently representable by MPS, leading to a rapid (typically exponential) growth of the bond dimension. If the bond dimension of the wavefunction is not dynamically adjusted to accommodate the growing correlations in the wavefunction the dynamics quickly becomes approximate and nonunitary. It is possible to construct a unitary time-propagation scheme on the manifold of MPS with a fixed bond dimension using the Dirac-Frenkel time-dependent variational principle (TDVP) [3–6]. This principle, which is rather generic, projects an infinitesimal time evolution under the Hamiltonian to a variational manifold which the resulting wavefunction is restricted to occupy. An advantage over conventional DMRG techniques is that the TDVP can be applied to a more general class of states, such as tree tensor network states, thus potentially opening the door to efficiently simulating higher dimensional systems as well as systems with long-ranged interactions.

The description of transport properties requires the investigation of large system sizes and long times, a limit which is sometimes referred to as the hydrodynamic limit. While this limit appears to be out of reach for numerically exact methods, an approximate coarse-grained treatment might be sufficient to obtain accurate macroscopic observables like transport coefficients, analogous to the success of classical hydrodynamics. In this respect the TDVP is particularly attractive, since it generates effectively chaotic classical dynamics in the space of variational parameters which obey a set of macroscopic conservation laws, such as those associated with the total number of particles and the total energy [7]. Indeed, a surprisingly fast convergence of the heat diffusion constant with respect to bond dimension has been very recently reported for a nonintegrable spin chain [8].

In this work, we examine the applicability of TDVP for the long time description of quantum interacting systems. While the method cannot be expected to work for quantum integrable systems (c.f. generalization of hydrodynamic approaches to such systems [9]), by utilizing the exact solvability of such systems we show that the long time limit, which is necessary to obtain hydrodynamic observables, and the large bond-dimension limit, where the method becomes numerically exact, do *not* generically "commute." In particular, the apparent convergence of hydrodynamic observables with the bond dimension does *not* guarantee the accuracy of the result, which has to be established by other means. This problem persists also for nonintegrable systems, although for the case of a disordered *nonintegrable* quantum system that we consider, this problem appears to be ameliorated.

Theory.— The Hilbert-space dimension of a quantum lattice systems scales exponentially with the size of the system. Any wavefunction in the Hilbert space can be written as a matrix product state (MPS),

$$|\Psi[A]\rangle = \sum_{\{s_n\}=1}^{d} A^{s_1}(1)A^{s_2}(2)\dots A^{s_N}(N)\,|s_1 s_2 \dots s_N\rangle \tag{1}$$

where d is the local Hilbert space dimension, $A^{s_i}(i) \in \mathbb{C}^{D_{i-1}\times D_i}$ are complex matrices and $D_0 = D_N = 1$, such

that the product of matrices evaluates to a scalar coefficient for a given configuration $|s_1 s_2 \dots s_n\rangle$. To be an *exact* representation of the wavefunction the dimension of the matrices the bond dimension must scale exponentially with the systems size. Typically one approximates the wavefunction by truncating the dimension of the matrices to a predetermined dimension with computationally tractable number of parameters. Exact results are obtained when the approximate dynamics are converged with respect to the bond dimension.

The time-dependent variational principle (TDVP) allows one to obtain a locally optimal (in time) evolution of the wavefunction on the manifold of MPS, $\mathcal{M}_{\mathbf{r}}$, with some fixed bond dimension $\mathbf{r}$. It amounts to solving a tangent-space projected Schrödinger equation [6]:

$$\frac{d\,|\Psi[A]\rangle}{dt} = -\mathrm{i} P_{\mathcal{M}} \hat{H}\,|\Psi[A]\rangle\,, \tag{2}$$

where $P_{\mathcal{M}}$ is the tangent space projector to the manifold $\mathcal{M}_{\mathbf{r}}$. Equation (2) is solved using a Trotter-Suzuki decomposition of the projector(see Ref. [6] for details).

The dynamics generated by the TDVP can be viewed as resulting from a classical, non-quadratic Lagrangian in the space of variational parameters [5, 8]. It can be shown that any conserved quantity of the Hamiltonian will be also conserved by TDVP if the corresponding symmetry group members of the associated quantity applied to a state in the manifold $\mathcal{M}_{\mathbf{r}}$ do not take it out of the manifold [7]. The nonlinearity of the equations of motion of TDVP disappears in the limit of infinite bond dimension, since in this limit the action of the Hamiltonian on the state keeps it on the manifold for all times.

Results.— We study transport properties of the one-dimensional XXZ model,

$$\hat{H} = J_{xy} \sum_{i=1}^{N-1} \left(\hat{S}_i^x \hat{S}_{i+1}^x + \hat{S}_i^y \hat{S}_{i+1}^y \right) + \Delta \sum_i \hat{S}_i^z \hat{S}_{i+1}^z + \sum_{i=1}^{N} h_i \hat{S}_i^z, \tag{3}$$

where h_i is uniformly distributed in the interval $[-W, W]$ and $\hat{S}_i^{(x,y,z)}$ are the appropriate projections of the spin operators on site i. In the following, we use $J_{xy} = 1$, which sets the time unit of the problem. Using the Jordan-Wigner transformation the XXZ model can be mapped to a model of spinless fermions [10]. For $\Delta = 0$, the corresponding model is noninteracting and can be solved exactly. In particular for $W \neq 0$ the system becomes Anderson localized [11]. For $\Delta \neq 0$ and at sufficiently high disorder the system becomes many-body localized and exhibits a dynamical phase transition [12, 13] which, for $\Delta = 1$, occurs at $W \approx 3.5$ [14, 15].

To study the dynamical properties of this model in its various limits we calculate the spreading of a spin-excitation as a function of time,

$$\sigma^2(t) = \sum_{i=1}^{L} (\frac{L}{2} - i)^2 \left\langle \hat{S}_i^z(t) \hat{S}_{L/2}^z(0) \right\rangle. \tag{4}$$

Here the expectation value is calculated at infinite temperature, namely $\left\langle \hat{O} \right\rangle = \mathrm{Tr}\, \hat{O}/\mathcal{N}$ where $\mathcal{N}$ is the Hilbert space dimension. The spread of the excitation is analogous to the classical mean-square displacement (MSD). Transport is characterized by assuming a power law scaling of the MSD, $\sigma^2(t) \sim t^\alpha$. For example, a dynamical exponent of $\alpha = 2$ ($\alpha = 1$) indicates ballistic (diffusive) transport. A dynamical exponent $0 < \alpha < 1$ corresponds to subdiffusive transport, and $\alpha = 0$ for localized systems. We also define a time-dependent diffusion constant $D(t)$ as the time-derivative of $\sigma^2(t)$ [16–19]. Throughout this work the hydrodynamic variable that we will consider will be the asymptotic spin diffusion coefficient, $\lim_{t\to\infty} D\,(t) \to D$.

To calculate the MSD we numerically evaluate the correlation function starting from a random configuration of up and down spins and also a random configuration of the disordered field, when appropriate. By sampling simultaneously both spin configurations and disorder configurations we obtain the required infinite temperature initial conditions and disorder average. The size of the system is chosen to be $L = 100 - 200$, such that all finite size effects are negligible on the simulated time scales, and the averages are obtained using at least 100 realizations.

The integration time-step is chosen such that no qualitative influence on the MSD is observed. For the models studied in this work time-steps of $0.05 - 0.2$ were found to satisfy this criterion. Because of the nonlinearity introduced in Eq. (2) due to $P_{\mathcal{M}}$, chaos emerges on a timescale, dubbed the Lyapunov time, which depends both on the bond-dimension, the realization studied, and the parameters of the system. Beyond this time, it becomes exponentially expensive (in time) to obtain convergence of the results on the level of *individual* configurations. We note in passing, that the Lyapunov time becomes longer for larger bond dimension [8].

To assess the convergence of the method, for each configuration determined by the initial configuration of the spins and the disorder configuration, we calculate the convergence time, $t_*\,(\omega)$ (here ω designates the configuration). For times $t < t_*\,(\omega)$ the dynamics generated starting from a given configuration is converged within a required accuracy (2%) by increasing the bond dimension. For the infinite temperature initial condition we use in this work, the convergence time, t_*, is calculated by averaging $t_*\,(\omega)$. It is crucial to consider *individual* configurations to assess the numerical convergence of the method since averaging over realizations introduces a fortuitous cancellation of errors, thus while t_* demarcates a strict, well-defined convergence metric, apparent convergence of either transport coefficients or dynamics may occur *after* this time. The averaged convergence times for which TDVP is numerically exact are comparable to convergence times of conventional DMRG or MPS techniques.

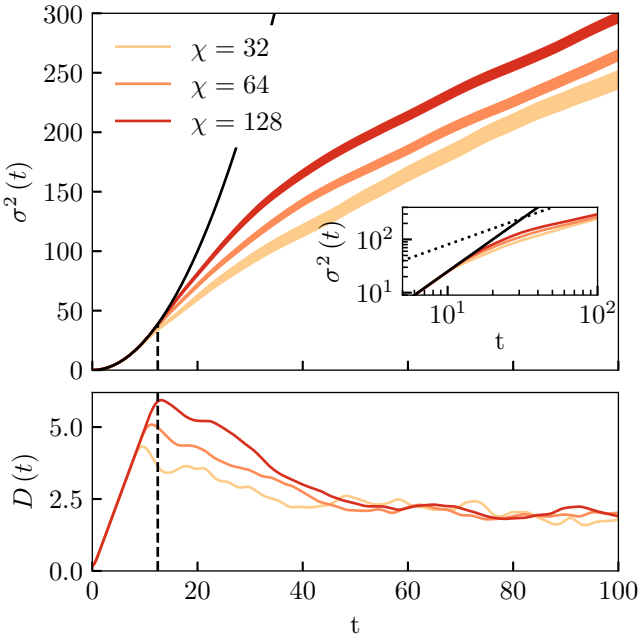

Figure 1. Clean XX model ($\Delta = 0$, $W = 0$). Upper panel: MSD as a function of time for various bond dimensions (32, 64, 128) averaged over 200-500 realizations of initial spin configurations and disorder. More intense shades represent larger bond dimensions and shaded areas indicate the standard-deviation of the observables obtained using a bootstrap procedure. The black solid line is an exact solution, obtained numerically. The inset shows the log-log scale of the main panel with the black dotted corresponding to diffusion. Lower panel: Time-dependent diffusion constant $D(t)$. The dashed black line on both plots represents the convergence time, t_*.

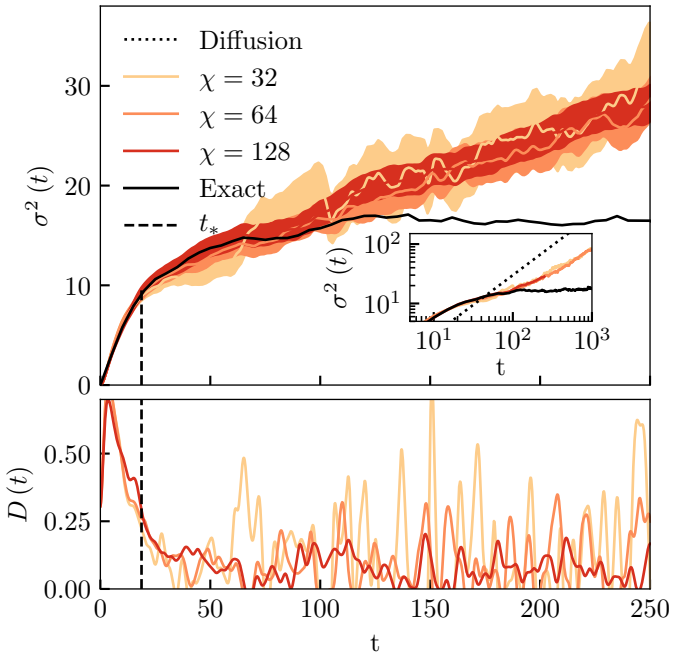

Figure 2. Same as Fig. (1) but for the disordered XX model ($\Delta = 0$, $W = 1$) for 100 realizations of initial spin configurations and disorder.

We first demonstrate that the long time limit essential for the study of hydrodynamics properties and the large bond-dimension limit, when the method becomes exact, do not "commute," in the sense that spurious, apparently converged long time behavior may emerge. For this purpose we will first consider two integrable models with a known dynamical behavior. We stress that true hydrodynamic behavior (at least in the usual sense) is *not* expected for such models.

Ballistic regime ($\Delta = 0$, $W = 0$, $L = 200$). The expected ballistic transport is accurately reproduced only up to $t_* \backsimeq 12$ for the largest bond-dimension employed (see Fig. 1). While this system corresponds to free fermions, the entanglement still grows limiting the accessible times. Beyond the convergence time transport appears to be diffusive with a diffusion constant of approximately 2.0. There is little variation of this value across the different bond-dimensions.

Anderson localized regime ($\Delta = 0$, $W = 1$, $L = 150$). This system is also effectively noninteracting with a MSD which saturates in time, indicating localization. TDVP fails to reproduce the plateau for all studied bond dimen-

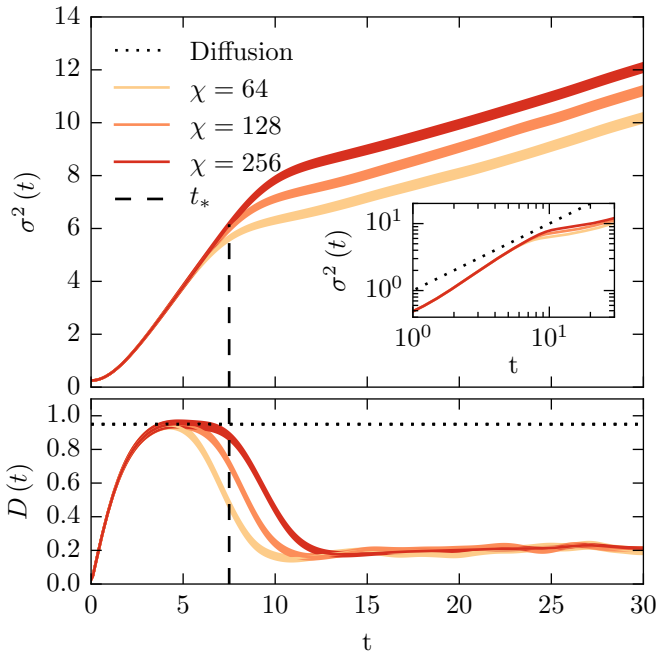

Figure 3. Same as Fig. (1) but for clean XX ladder of length $L = 50$ with isotropic coupling between the rungs. The results were obtained by averaging 100 realizations of initial spin configurations. The black dotted line in the bottom panel represents the previously reported diffusion constant [20].

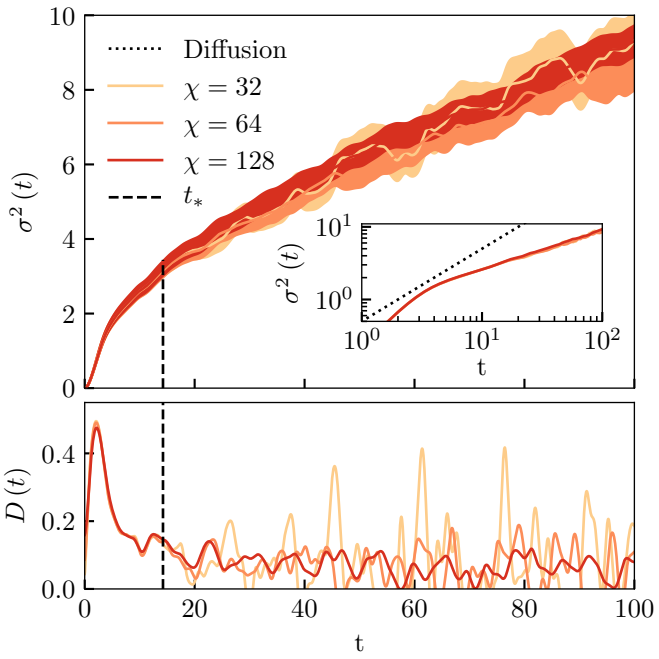

Figure 4. Same as Fig. (1) but for disordered XXZ model in the subdiffusive regime ($\Delta = 1$, $W = 1.5$) for 200 realizations of initial spin configurations and disorder.

sions and displays growth of the MSD with time although the diffusion coefficient is rather small (see Fig. 2). Results obtained using the largest bond-dimension (128) follow the exact result closely up to about $t = 70$, while those of smaller bond-dimensions deviate significantly earlier, resulting in $t_* = 19$.

Since asymptotically the nonlinear equations of TDVP are expected to result in diffusion, the striking failure of the method for the two integrable systems above is not surprising.

Diffusive XX-ladder ($\Delta = 0$, $L = 50$). This model is a generalization of (3) to a two leg ladder. It is nonintegrable and shows convincing diffusion with a diffusion coefficient of about $D \sim 0.95$ [20, 21]. As expected for short times the calculations based on the TDVP reproduce this numerically exact results (see Fig. 3) However, for times longer than the convergence time, $t > t_* = 8$, a crossover to yet another diffusive regime with much lower diffusion constant appears ($D \sim 0.2$). Moreover this diffusion coefficient does not appear to strongly depend on the bond-dimension.

The above examples illustrate that the seemingly converged transport coefficients and long time dynamics within the TDVP framework can be highly misleading. After demonstrating the pitfalls in determining the long-time properties using TDVP, we examine its potential as a hydrodynamic method for a disordered nonintegrable system.

Subdiffusive regime ($\Delta = 1.0$, $W = 1.5$, $L = 100$). For moderate disorder $0 < W < 3.7$ the system is nonintegrable [19]. While the convergence time here is about $t_* = 18$, semi-quantatively similar subdiffusive transport appears also at much longer times (see inset in Fig. 4). Interestingly, the exponent extracted from the long-time behavior, $\alpha = 0.54$, is in excellent agreement with previously reported value, extracted from the short time dynamics of the same system using exact diagonalization [19, 22–24]. This indicates that for such a system, true asymptotic dynamical behavior may indeed be uncovered using moderate numerical costs (small bond-dimensions).

Discussion.— In this work we have examined how well TDVP captures the *long time* behavior of quantum interacting systems. For any *finite* time the method is formally numerically exact, since it can be converged with respect to the bond dimension and other numerical parameters. For longer times convergence cannot be guaranteed generically, but one hopes that *on average* the method will still produce the correct result, due to ergodicity of the TDVP trajectories on the MPS manifold. This assumes that the MPS ansatz captures all the relevant local correlations that produce long time behavior.

By examining integrable and nonintegrable models for which the asymptotic dynamics in known, we have shown that the apparent convergence of long time observables, such as the diffusion coefficient, obtained using TDVP is *not* indicative of the accuracy of the method and may be very misleading. While the dramatic failure of TDVP to reproduce ballistic and localized dynamics is expected, it is quite unfortunate that the method appears to fail also for a nonintegrable diffusive model.

Interestingly, the most promising results are obtained for the nonintegrable *disordered* XXZ model in the ergodic subdiffusive phase [19], which is the only presented example where the short time and long time behavior appear to agree very well, although the same caveats concerning convergence apply. This is quite surprising, in light of the expectation of asymptotic diffusion in TDVP generated dynamics due to the underlying nonlinearity of the equations of motion. Nevertheless, we find that the MSD calculated by TDVP is strongly sublinear, although we cannot rule out a slow approach of the dynamical exponent to its diffusive value. We would like to point out a possible connection between the nonlinearity introduced by the tangent space projector into the TDVP equations of motion and the nonlinear dependence on the wave function in the self-consistent second Born approximation, [12, 25, 26] and the nonlinear Schrödinger equation (NLSE), both of which also show subdiffusive transport in the presence of disorder [27].

In summary, we have shown that great care must be exercised examining the apparent convergence of long time properties within the TDVP approach, which appears to generically produce either qualitatively or quantitatively incorrect results. Nevertheless, we have presented

one nontrivial system were the short time (numerically exact) dynamics and the long time dynamics agree, and therefore hint at the possibility of an accurate asymptotic description, obtained at a modest computational effort. It is of great importance to further investigate the origins of the apparent success of the method in this case as well as to extend this study to other nonintegrable systems in one and two-dimensions.

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