Comment on "Time-Dependent Density-Matrix Renormalization Group: A Systematic Method for the Study of Quantum Many-Body Out-of-Equilibrium Systems"

In a recent Letter [1], Cazalilla and Marston (CM) proposed a time-dependent density-matrix renormalization group (TdDMRG) algorithm for studies of out-of-equilibrium properties of quantum many-body systems. An interesting result they obtained is that for a tunneling junction of two Luttinger liquids, a current oscillation develops after initial transient in the insulating regime (Fig. 2 in Ref. [1]). They attributed this oscillation to a nonlinear response of the Luttinger liquid. Here we comment that (i) the oscillation they observed is an artifact of the method, and (ii) the TdDMRG can be significantly improved by extending the definition of the density matrix to adapt the nonequilibrium evolution of the ground state.

In the TdDMRG scheme of CM, it is the equilibrium ground state $|\Psi_0\rangle$ that is used for the construction of the reduced density matrix. At the beginning of the evolution, the state does not deviate much from $|\Psi_0\rangle$, and the results are accurate. However, the time evolution of $|\Psi_0\rangle$ evokes excited states in a nonequilibrium system, so its long time behavior becomes very poor and could not be substantially improved by keeping more states. This can be clearly seen from Fig. 1, where the numerical results obtained with CM's approach (i.e., the $N_t = 0$ curves) for the two models in Ref. [1] begin to deviate from the exact ones at $t \sim 25$.

To retain the information on the relevant excitation states, we propose to define the density matrix from the time-dependent wave function $|\Psi(t)\rangle$ as

$$\rho = \sum_{i=0}^{N_t} \alpha_i |\Psi(t_i)\rangle\langle\Psi(t_i)|, \qquad \sum_i \alpha_i = 1, \tag{1}$$

where $|\Psi(t_0)\rangle = |\Psi_0\rangle$, t_0 is the time at which a bias is imposed and N_t is the number of equal time intervals within the whole evolution time to be evaluated for each length L. The reduced density matrix for the system is defined by tracing over the degrees of freedom of the environment. Both $|\Psi(t)\rangle$ and the newly defined reduced density matrix should be evaluated at each density-matrix renormalization group (DMRG) step from the beginning of the truncations, not just for the final lattice system. Moreover, at each step of the DMRG the same time-dependent bias voltage is applied. The density matrix of CM corresponds to the $N_t = 0$ case. In our calculation, we took $\alpha_i = 1/2$ for $i = 0$ and $1/2N_t$ otherwise. Empirically, we find that $N_t \geq 6$ is generally needed. Figure 1 shows our results with $N_t = 24$. By comparison with the exact results, we find that this new scheme can significantly improve the large time scale behavior of the current.

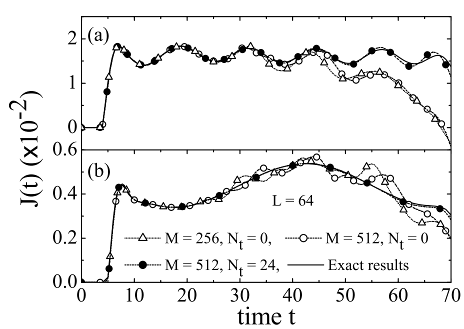

FIG. 1. Current for (a) a quantum dot and (b) a junction with $V = 0$, defined by Eqs. (2) and (5) in Ref. [1], respectively.

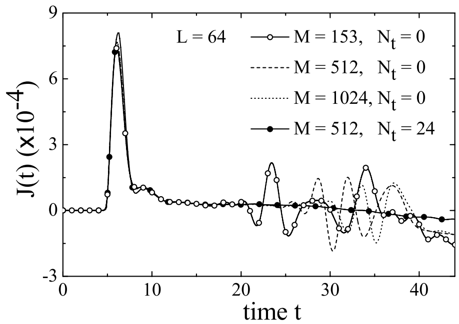

FIG. 2. Tunneling current for the model defined by Eq. (5) in Ref. [1] with $V = 1.1w$ and $\delta\mu = 6.25 \times 10^{-2}w$.

Now let us turn to the tunneling junction between two Luttinger liquids in the insulating regime. For $N_t = 0$, our calculation confirms the existence of a current oscillation around $t \sim 20$. However, we find that the oscillation depends on the number of states retained. By further applying the new TdDMRG scheme to this system, we find that the oscillation does not exist at all. In Fig. 2 the numerical results with $N_t = 0$ and $N_t = 24$ are shown for detailed comparisons. Therefore, the current oscillation observed by CM is in fact an artifact of the TdDMRG [1], rather than a nonlinear response of the system to the applied bias. This also shows that, in the study of physical properties of a quantum state out of equilibrium, it is important to include the relevant excitation states in the definition of the reduced density matrix.

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[1] M. A. Cazalilla and J. B. Marston, Phys. Rev. Lett. **88**, 256403 (2002).

