Regression Relation for Pure Quantum States and Its Implications for Efficient Computing

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Regression relation for pure quantum states and its implications for efficient computing

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We obtain a modified version of the Onsager regression relation for the expectation values of quantum-mechanical operators in pure quantum states of isolated many-body quantum systems. We use the insights gained from this relation to show that high-temperature time correlation functions in many-body quantum systems can be controllably computed without complete diagonalization of the Hamiltonians, using instead the direct integration of the Schroedinger equation for randomly sampled pure states. This method is also applicable to quantum quenches and other situations describable by time-dependent many-body Hamiltonians. The method implies exponential reduction of the computer memory requirement in comparison with the complete diagonalization. We illustrate the method by numerically computing infinite-temperature correlation functions for translationally invariant Heisenberg chains of up to 29 spins 1/2. Thereby, we also test the spin diffusion hypothesis and find it in a satisfactory agreement with the numerical results. Both the derivation of the modified regression relation and the justification of the computational method are based on the notion of quantum typicality.

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In 1931, Onsager came up with the profound insight that "the average regression of fluctuations will obey the same laws as the corresponding macroscopic irreversible process"[1]. This regression relation became the cornerstone of the linear response theory. From today's perspective, Onsager's regression relation (ORR) is equivalent[2,3] to the high-temperature limit of the fluctuation-dissipation theorem[4]. In this paper, we show that a modified version of ORR holds for the expectation values of quantum-mechanical operators, when a many-body system is in a pure quantum state. We also present an efficient method for computing high-temperature linear response characteristics of many-particle quantum systems using the time evolution of a single pure state.

There exists a class of nonperturbative problems, such as nuclear spin-spin relaxation in solids[5], where the relaxation or correlation functions in translationally-invariant systems need to be computed at high temperatures. Despite the progress in the approximate methods, e.g.[6,7], and numerical techniques[8–11], the above kind of problems generally resist *controllable* solutions, leaving the complete diagonalization of quantum Hamiltonians as the only way to obtain controllable results. The sizes of the systems treatable by complete diagonalization are severely limited by the computer memory requirement that scales as N^2, where N is the number of quantum states in the system. The memory requirement for the controllable-accuracy algorithm proposed in this work scales at most a $N(\log N)^2$.

In recent years, it was realized that, given the exponentially large number N of quantum states in a many-particle system, many observable properties of such a system can be obtained by sampling one suitably chosen pure quantum state, or a wave function — the so-called "quantum typicality"[12–16]. In particular, Refs.[7,17–19] applied the notion of quantum typicality to the relaxation and fluctuation phenomena, but on the numerical side these investigations dealt so far only with the systems that were sufficiently small, so that a complete diagonalization of the Hamiltonian could have been done, if desired.

In this paper, we report a conceptual and a computational results, which are both connected to the notion of typicality but, otherwise, only indirectly connected to each other. The conceptual result is that the expectation values of quantum-mechanical operators in a *pure* quantum state obey the usual regression relation but with the amplitude of fluctuations exponentially reduced in comparison with the classical case (see Eq.(8) below). The computational result is that the high-temperature time correlation functions of both local and extensive quantities can be controllably computed on the basis of Eq.(9) without complete diagonalization of the Hamiltonians, using instead the direct integration of the Schrödinger equation for randomly sampled pure states. As an example, we obtain infinite-temperature correlation functions for translationally invariant Heisenberg chains of up to 29 spins 1/2, thereby also testing the spin diffusion hypothesys. To the best of our knowledge, none of the complete diagonalization studies of the Heisenberg spin-1/2 chains conducted so far has reached the above size. We note here that pure quantum states were used in Refs.[20,21] in the context of other numerical methods.

Below, in order to be specific, we consider a lattice of N_s interacting spins 1/2 with the total number of quantum states $N = 2^{N_s} \gg 1$ and the Hamiltonian $\mathcal{H}$. We adopt the following conventions: (i) Analytical formulas are presented only in the leading order in $1/N$. (ii) Wave functions without time argument and operators with time argument imply the Heisenberg representation of quantum mechanics. The opposite implies the Schrödinger representation. (iii) $\hbar = 1$.

We now focus on some observable quantity, e.g. total spin polarization, characterized by operator $\hat{A} \equiv A_{mn}$, which has zero average value at the infinite-temperature equilibrium, i.e. $\mathrm{Tr}\{\hat{A}\} = 0$. The Onsager regression relation for this quantity near the infinite temperature equilibrium has the following form:

$$\mathrm{Tr}\left\{\hat{A}(t)\rho_{\mathrm{neq}}\right\} = \frac{\alpha}{N}\mathrm{Tr}\left\{\hat{A}(t)\hat{A}(0)\right\}. \tag{1}$$

where $\hat{A}(t) = e^{i\mathcal{H}t}\hat{A}e^{-i\mathcal{H}t}$, and $\rho_{\mathrm{neq}} = \frac{1}{N}\exp(\alpha\hat{A})$ with α being a small constant. The right-hand side (RHS) of Eq.(1) represents the equilibrium time correlation function of $\hat{A}$, while the left-hand side (LHS) is the relaxation function of $\hat{A}$ corresponding to the initial nonequilibrium density matrix ρ_{neq}. A detailed discussion of Eq.(1) and its relation to the fluctuation-dissipation theorem is given in Ref.[22].

Quantum typicality investigation of Ref.[18] implied that

$$\langle\Psi_{\mathrm{neq}}|\hat{A}(t)|\Psi_{\mathrm{neq}}\rangle = \mathrm{Tr}\left\{\hat{A}(t)\rho_{\mathrm{neq}}\right\}\left[1 + O\left(\frac{1}{\alpha\sqrt{N}}\right)\right], \tag{2}$$

where $|\Psi_{\mathrm{neq}}\rangle$ is a wave function that "samples" ρ_{neq}.

Now we obtain a complementary relation on the fluctuation side. It involves the wave function $|\Psi_{\mathrm{eq}}\rangle$ representing the infinite temperature equilibrium and defined as a random vector in the Hilbert space of the system. $|\Psi_{\mathrm{eq}}\rangle$ can be generated in *any* orthonormal basis $\{|\phi_k\rangle\}$ as follows:

$$|\Psi_{\mathrm{eq}}\rangle = \sum_{k=1}^{N} a_k|\phi_k\rangle, \tag{3}$$

where a_k are the quantum amplitudes, whose absolute values are selected from the probability distribution[23,24]

$$P(|a_k|^2) = N\exp(-N|a_k|^2) \tag{4}$$

and the phases are chosen randomly in the interval $[0, 2\pi)$. In the following, we use bar above an expression to indicate the Hilbert-space average over all possible choices on $|\Psi_{\mathrm{eq}}\rangle$.

Now we consider the correlation function for the time series of the expectation value $\langle\Psi_{\mathrm{eq}}|\hat{A}(t')|\Psi_{\mathrm{eq}}\rangle$ in the time interval $[-T_0, T_0 + t]$:

$$C(t, T_0) \equiv \frac{1}{2T_0}\int_{-T_0}^{T_0} dt' \langle\Psi_{\mathrm{eq}}|\hat{A}(t + t')|\Psi_{\mathrm{eq}}\rangle\langle\Psi_{\mathrm{eq}}|\hat{A}(t')|\Psi_{\mathrm{eq}}\rangle. \tag{5}$$

In[22], we derive the following relation:

$$C(t, T_0) = \frac{1}{N^2}\mathrm{Tr}\left\{\hat{A}(t)\hat{A}(0)\right\} + \Delta_1, \tag{6}$$

where

$$\overline{\Delta_1^2} \approx \frac{1}{2\sqrt{2}\ T_0 N^4}\int_{-T_0\sqrt{2}}^{T_0\sqrt{2}} dt_2 \left(\left[\mathrm{Tr}\left\{\hat{A}(t_2)\hat{A}(0)\right\}\right]^2 + \mathrm{Tr}\left\{\hat{A}(t - t_2)\hat{A}(0)\right\}\mathrm{Tr}\left\{\hat{A}(t + t_2)\hat{A}(0)\right\}\right). \tag{7}$$

For large enough T_0, the correction Δ_1 in Eq.(6) is much smaller than the principal term as long as $\mathrm{Tr}\left\{\hat{A}(t)\hat{A}(0)\right\} \xrightarrow{t\to\infty} 0$. In particular, if $\mathrm{Tr}\left\{\hat{A}(t)\hat{A}(0)\right\}$ decays at large t faster than $|t|^{-0.5}$ then, for large enough T_0, the integral in Eq.(7) becomes independent of T_0, and, as a result, $\Delta_1 = O(\sqrt{\tau/T_0})\mathrm{Tr}\left\{\hat{A}^2\right\}/N^2$, where τ is the characteristic timescale for the decay of the expression under the integral. If $\mathrm{Tr}\left\{\hat{A}(t)\hat{A}(0)\right\}$ decays asymptotically as $|t|^{-\nu}$ with $0 < \nu < 0.5$, then, according to Eq.(7), Δ_1 still remains small, but its prefactor scales as $O(T_0^{-\nu})$. The condition $\mathrm{Tr}\left\{\hat{A}(t)\hat{A}(0)\right\} \xrightarrow{t\to\infty} 0$ is overwhelmingly likely to be fulfilled for physical observables (local or extensive) in generic nonintegrable quantum systems. However, the violation of this condition should be suspected and investigated on case-by-case basis in integrable systems or in disordered systems exhibiting tendency towards many-body localization.

We note that the leading term in the RHS of Eq.(6) was obtained in Ref.[19] for a slow Markovian variable $\hat{A}$ with exponentially decaying correlation function. This result was based on the quantum ergodicity conjecture, which allowed the authors to substitute the RHS of Eq.(5) with the Hilbert space average of $\langle\Psi_{\mathrm{eq}}|\hat{A}(t+t')|\Psi_{\mathrm{eq}}\rangle\langle\Psi_{\mathrm{eq}}|\hat{A}(t')|\Psi_{\mathrm{eq}}\rangle$. In comparison, we directly derived both the leading term and the correction in Eq.(6) for a single realization of the time series of $\langle\Psi_{\mathrm{eq}}|\hat{A}(t)|\Psi_{\mathrm{eq}}\rangle$ without relying on the ergodicity conjecture. In addition, our treatment does not restrict $\hat{A}$ to be a slow Markovian variable[22].

Eq.(6) together with Eqs.(1,2) implies the modified version of ORR for the expectation value of the operator $\hat{A}$ in a pure quantum state:

$$\lim_{N\to\infty}\langle\Psi_{\mathrm{neq}}|\hat{A}(t)|\Psi_{\mathrm{neq}}\rangle = \alpha \lim_{T_0\to\infty, N\to\infty} NC(t,T_0), \tag{8}$$

where, in the RHS, the limit $N \to \infty$ is taken first, which in practical terms means that T_0 should be much smaller than the inverse spacing of the energy levels in the system as the above limits are taken[22].

From the viewpoint of practical computing, the implications of the above findings are two-fold: (i) As already implicit in Eq.(2), and explicit in Eqs.(6,8), a single realization of $\langle\Psi_{\mathrm{neq}}|\hat{A}(t)|\Psi_{\mathrm{neq}}\rangle$ is exponentially more accurate in approximating $\mathrm{Tr}\left\{\hat{A}(t)\hat{A}(0)\right\}$ than the corresponding single classical relaxation process in approximating classical correlation function[22]. $\langle\Psi_{\mathrm{neq}}|\hat{A}(t)|\Psi_{\mathrm{neq}}\rangle$ decays into the equilibrium statistical noise $\langle\Psi_{\mathrm{eq}}|\hat{A}(t)|\Psi_{\mathrm{eq}}\rangle$, which, according to Eq.(6) has root-mean-squared (rms) amplitude $\sqrt{C(0,T)} \approx \sqrt{\mathrm{Tr}\{\hat{A}^2\}}/N$, which is by factor of $\sqrt{N}$ smaller than the rms amplitude $\sqrt{\mathrm{Tr}\{\hat{A}^2\}/N}$ expected for the classical noise or the noise of continuously monitored macroscopic quantum observable at infinite temperature[22,25]. This noise suppression is due to the fact that the time evolution of a single pure state contains the superposition of N independent "noises" associated with each of the basis states[17]. The statistical noise of $\langle\Psi_{\mathrm{neq}}|\hat{A}(t)|\Psi_{\mathrm{neq}}\rangle$ can be suppressed further by averaging over many pure-state evolutions. (ii) In principle, as we show below, the direct evaluation of $C(t,T)$ can also be used to obtain $\mathrm{Tr}\left\{\hat{A}(t)\hat{A}(0)\right\}$, but this procedure does not take advantage of the above-mentioned quantum parallelism and hence is less efficient.

Although the evaluation of $\langle\Psi_{\mathrm{neq}}|\hat{A}(t)|\Psi_{\mathrm{neq}}\rangle$ is a very efficient method to obtain $\mathrm{Tr}\left\{\hat{A}(t)\hat{A}(0)\right\}$, an even more efficient method is to use typicality to sample this trace directly on the basis of the following relation anticipated in[12] and derived in[22]:

$$\langle\Psi_{\mathrm{eq}}|\hat{A}(t)\hat{A}(0)|\Psi_{\mathrm{eq}}\rangle = \frac{1}{N}\mathrm{Tr}\left\{\hat{A}(t)\hat{A}(0)\right\} + \Delta_2, \tag{9}$$

where

$$\overline{\Delta_2^2} = \frac{1}{N^2}\mathrm{Tr}\left\{\hat{A}(t)\hat{A}(0)\hat{A}(t)\hat{A}(0)\right\}. \tag{10}$$

That the second term in the RHS of Eq.(9) is much smaller than the first one can be shown by estimating their ratio at $t = 0$ as $\frac{\sqrt{\mathrm{Tr}\{\hat{A}^4\}}}{\mathrm{Tr}\{\hat{A}^2\}} \sim \frac{1}{\sqrt{N}}$. The statistical accuracy of computing $\mathrm{Tr}\left\{\hat{A}(t)\hat{A}(0)\right\}$ with the help of Eq.(9) is thus better by factor $1/\alpha$ in comparison with Eq.(2).

In Fig.1 we demonstrate the relationships (2, 6, 9) by computing the intermediate dynamic structure factor $I_\pi(t)$ for the Heisenberg chain of 20 spins 1/2 using complete diagonalization. Thereby we also demonstrate the regression relation (8). The Hamiltonian of this chain is $\mathcal{H} = J\sum_i \mathbf{S_i}\cdot\mathbf{S_{i+1}}$ with periodic boundary condition. Here J is the coupling constant, and $\mathbf{S_i}$ is the spin operator on the ith chain site. Such a chain admits periodic spin modulations with wave numbers $q = 2\pi n/N_s$, where n is an integer number taking values $0, 1, ..., N_s - 1$. For a given wave number q, the intermediate dynamic structure factor is defined as

$$I_q(t) \cong \mathrm{Tr}\left\{\hat{A}_{\{q\}}(t)\ \hat{A}_{\{q\}}(0)\right\}, \tag{11}$$

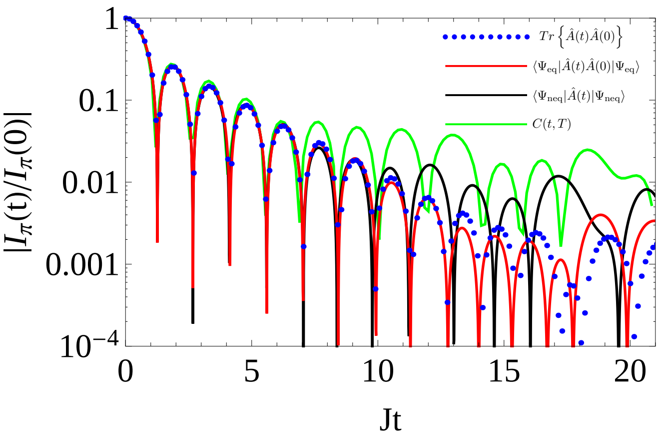

FIG. 1: Intermediate dynamic structure factor $I_\pi(t)$ of the Heisenberg chain of 20 spins 1/2. The calculation based on the exact trace formula (11) is compared with the approximations given by Eqs.(2,6,9) as indicated in the legend. The initial agrement between the black and the green lines also demonstrates the validity of the regression relation (8). All calculations are based on the complete diagonalization of the Hamiltonian $\mathcal{H}$. Each of the three approximate calculations is done with a single pure state. In the case of Eq.(2), $\alpha = 0.083$ corresponding to the initial polarization equal to approximately 4 percent of the maximum polarization. In the case of Eq.(6), $T = 4200/J$. As expected theoretically, the approximation based on Eq.(9) gives the most accurate agreement with the exact result. (Note the logarithmic vertical scale.) The accuracy of all three approximations can be improved by averaging over more pure states.

where $\hat{A}_{\{q\}} = \sum_m \cos(qm) S_m^x$.

Now, we proceed with showing that, for the spin systems too large to be treated by complete diagonalization, it is still possible to controllably compute infinite temperature correlation functions by evaluating the LHS of Eq.(9) with the help of the direct integration of the Schrödinger equation.

We compute the time evolution of pure states on the basis of the time-discretized version of the Schrödinger equation. We use the fourth-order Runge-Kutta routine[26] based on the following equation:

$$|\Psi(t+\Delta t)\rangle = |\Psi(t)\rangle + |v_1\rangle + |v_2\rangle + |v_3\rangle + |v_4\rangle, \tag{12}$$

where Δt is the discretization time step, and $|v_1\rangle, |v_2\rangle, |v_3\rangle, |v_4\rangle$ are unnormalized Hilbert-space vectors computed as follows: $|v_1\rangle = -i\mathcal{H}|\Psi(t)\rangle\Delta t$, $|v_2\rangle = -\frac{1}{2}i\mathcal{H}|v_1\rangle\Delta t$, $|v_3\rangle = -\frac{1}{3}i\mathcal{H}|v_2\rangle\Delta t$, and $|v_4\rangle = -\frac{1}{4}i\mathcal{H}|v_3\rangle\Delta t$. Given the linearity of the Schrödinger equation, Eq.(12) is equivalent to the simple 4th order power-series expansion of the time-evolution operator at each discretization time step. We used $\Delta t = 0.01/J$

The above routine requires only storing in the memory the vectors $|\Psi\rangle$ and $|v_i\rangle$ and the non-zero elements of the Hamiltonian $\mathcal{H}$. Although the Hamiltonian is an $N \times N$ matrix, it is very sparse for many-particle systems with only two-particle interactions when represented in a "local" basis, where each basis function is factorizable in terms of the wave functions of individual particles. For N_s spins 1/2, a possible local basis is the one where the z-projections of all spins are quantized. In this basis, the number of the nonzero entries of the Hamiltonian matrix is of the order of $N \times N_s^2$ for the systems with long-range interactions, or $N \times N_s$ for the short range interactions. Thus the overall memory required for the direct propagation of the Schroedinger equation scales at most as $N(\log N)^2$, i.e. it is exponentially smaller than the memory required for the complete diagonalization, which scales as N^2. One can take advantage of this memory reduction only when the operator of interest, $\hat{A}$, is also sparse in the local basis, but this is normally the case in physical contexts. In fact, in many cases, including the calculations of $I_q(t)$, it is possible simply to use the eigenbasis of $\hat{A}$ as the local basis.

We verify the accuracy of the direct integration method in two ways. For small spin clusters, we compare the wave functions obtained by propagating the same initial state using either complete diagonalization or the direct integration method. As shown in Fig. 2(a), the overlap between the two wave functions remains extremely close to 1 over the time interval required to compute $I_\pi(t)$ for 20 spins 1/2 in Fig. 1. For larger systems, we compare two wave functions $|\Psi_1(t)\rangle$ and $|\Psi_2(t)\rangle$ obtained by propagating the same initial wave function using the direct integration method with two different discretization time steps Δt_1 and Δt_2 such that $\Delta t_2 = 2\Delta t_1$. We then verify that that their overlap $\langle\Psi_1(t)|\Psi_2(t)\rangle$ is sufficiently close to 1. An example of such a test for 29-spin Heisenberg chain is shown in Fig. 2(b).

We note here that the same direct integration algorithm can be used to compute the imaginary-time evolution associated with the expression $\exp(-\mathcal{H}\beta/2)|\Psi_{\rm eq}\rangle$, where β is the inverse temperature, thereby generating equilibrium

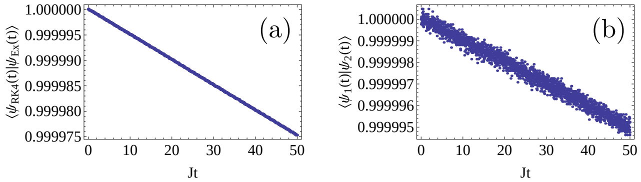

FIG. 2: Tests of numerical accuracy of the direct integration of the Schrödinger equation. (a) Overlap between two initially identical wave functions for the Heisenberg chain of 20 spins 1/2, $|\Psi_{\rm Ex}(t)\rangle$ and $|\Psi_{\rm RK4}(t)\rangle$, computed using, respectively, the complete diagonalization and the direct integration. (b) Overlap between two initially identical wave functions for the Heisenberg chain of 29 spins 1/2, $|\Psi_1(t)\rangle$ and $|\Psi_2(t)\rangle$, both computed using the direct integration method with two respective discretization time steps $\Delta t_1 = 0.01/J$ and $\Delta t_2 = 0.02/J$. The noisiness of the line originates from the accumulated machine rounding errors.

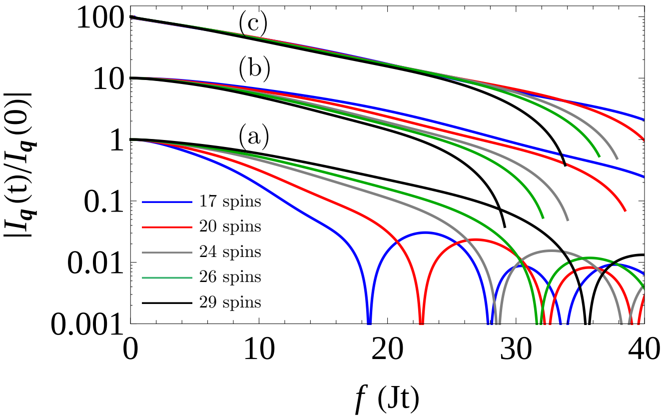

FIG. 3: Intermediate dynamic structure factors $I_q(t)$ for Heisenberg chains of N_s spins 1/2 computed as the LHS of Eq.(9) by propagating a single pure state with the help of the direct integration of the Schrödinger equation. The values of N_s are indicated in the plot legend. In each case, $q = 2\pi/N_s$. The horizontal axis is: (a) $f(Jt) = Jt$, (b) $f(Jt) = \xi_1 \; q^2 t$, and (c) $f(Jt) = \xi_2 \; q^2 \, (1 + 0.1 \; \ln q) \, t \ln t$, where ξ_1 and ξ_2 are arbitrary scaling parameters. The vertical axes for (b) and (c) are displaced for better visibility. Plots (a) represent the original calculation results. Plots(b) test the scaling expected for spin diffusion. Plots (c) test the empirical scaling reported for classical spins in Ref.[27]. The numerical accuracy test for the pure state evolution in the case of the 29-spin chain is given in Fig. 2(b).

wave function corresponding to temperature $1/\beta$. This wave function can then be used to compute the linear response characteristics at temperature $1/\beta$.

Our numerical procedure for computing $\langle\Psi_{\rm eq}|\hat{A}(t)\hat{A}(0)|\Psi_{\rm eq}\rangle$ is based on propagating two wave functions using the direct integration method[7]. One of them is $|\Psi_{\rm eq}(t)\rangle = \exp(-i\mathcal{H}t)|\Psi_{\rm eq}(0)\rangle$, where $|\Psi_{\rm eq}(0)\rangle$ is given by Eq.(3). The other one is $|\Phi(t)\rangle = \exp(-i\mathcal{H}t)|\Phi(0)\rangle$, where $|\Phi(0)\rangle = \hat{A}|\Psi_{\rm eq}(0)\rangle$ (i.e. $|\Phi(0)\rangle$ is unnormalized). The quantity of interest $\langle\Psi_{\rm eq}|\hat{A}(t)\hat{A}(0)|\Psi_{\rm eq}\rangle$ is then evaluated as $\langle\Psi_{\rm eq}(t)|\hat{A}|\Phi(t)\rangle$.

Now we exemplify the direct integration method by computing the intermediate dynamic structure factors $I_q(t)$ with $q = 2\pi/N_s$ for Heisenberg chains of sizes up to $N_s = 29$. By doing this calculation, we also test the spin diffusion hypothesis, which stipulates that, for sufficiently small values of q, $I_q^{\mu}(t) \approx e^{-Dq^2 t}$, where D is the diffusion coefficient.

Our results presented as plots (a) in Fig.3 indicate that, in every case, $I_q(t)$ shows the initial tendency to decay exponentially, but then the behavior universally starts exhibiting oscillations. Plots (b) in the same figure further indicate that the nearly exponential parts of $I_q(t)$ exhibit satisfactory q^2-scaling, while plots 2(c) show that the scaling $q^2(1 + 0.1 \; \ln q)\ln t$ reported in the numerical studies of classical spins[27] works even better. Overall, the above results appear to be consistent with recent investigations[28,29] suggesting that the isotropic Heisenberg chain of spins 1/2 is the border case for the transition between ballistic and diffusive behavior.

To summarize, we obtained the modified Onsager regression relation (8) for a pure quantum state. We also find that the direct computation of the LHS of Eq.(9) is the most efficient way to obtain equilibrium time correlation functions with controllable accuracy. We have directly tested only the high-temperature limit but the method itself can also be used at finite temperatures. We further note that the direct integration of the Schrödinger equation in combination with the random sampling of pure states can also be used for the efficient computing of quantum quenches and other situations describable by time-dependent many-body Hamiltonians.

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[1] L. Onsager, Phys. Rev. **38**, 2265 (1931).
[2] G. W. Ford and R. F. O'Connell, Phys. Rev. Lett. **77**, 798 (1996).
[3] M. Lax, Optics Communications **179**, 463 (2000).
[4] H. B. Callen and T. A. Welton, Phys. Rev. **83**, 34 (1951).
[5] A. Abragam, *Principles of Nuclear Magnetism* (Oxford University Press, Oxford, 1961).
[6] B. V. Fine, Phys. Rev. Lett. **79**, 4673 (1997).
[7] W. Zhang, N. Konstantinidis, K. A. Al-Hassanieh, and V. V. Dobrovitski, J. Phys. Condens. Matter **19**, 083202 (2007).
[8] F. Verstraete and J. Cirac, cond-mat/0407066 (2004).
[9] S. R. White and A. E. Feiguin, Phys. Rev. Lett. **93**, 076401 (2004).
[10] U. Schollwöck, Rev. Mod. Phys. **77**, 259 (2005).
[11] G. M. Crosswhite, A. C. Doherty, and G. Vidal, Phys. Rev. B **78**, 035116 (2008).
[12] A. Hams and H. De Raedt, Phys. Rev. E **62**, 4365 (2000).
[13] J. Gemmer, M. Michel, and G. Mahler, *Quantum Thermodynamics* (Springer Verlag, Berlin/Heidelberg, 2004).
[14] S. Goldstein, J. L. Leibowitz, R. Tumulka, and N. Zanghi, Phys. Rev. Lett. **96**, 050403 (2006).
[15] S. Popescu, A. J. Short, and A. Winter, Nature Physics **2**, 754 (2006).
[16] P. Reimann, Phys. Rev. Lett. **99**, 160404 (2007).
[17] G. A. Álvarez, E. P. Danieli, P. R. Levstein, and H. M. Pastawski, Phys. Rev. Lett. **101**, 120503 (2008).
[18] C. Bartsch and J. Gemmer, Phys. Rev. Lett. **102**, 110403 (2009).
[19] C. Bartsch and J. Gemmer, Europhys. Lett. **96**, 60008 (2011).
[20] M. W. Long, P. Prelovšek, S. El Shawish, J. Karadamoglou, and X. Zotos, Phys. Rev. B **68**, 235106 (2003).
[21] S. R. White, Phys. Rev. Lett. **102**, 190601 (2009).
[22] See the electronic supplemental material.
[23] B. V. Fine, Phys. Rev. E **80**, 051130 (2009).
[24] Here we neglect the normalization correction $|\Psi_{\rm eq}|^2 = 1 + O(1/\sqrt{N})$ associated with the statistical fluctuations of $|a_k|^2$.
[25] F. Bloch, Phys. Rev. **70**, 460 (1946).
[26] A. E. Feiguin and S. R. White, Phys. Rev. B **72**, 020404 (2005).
[27] O. F. de Alcantara Bonfim and G. Reiter, Phys. Rev. Lett. **69**, 367 (1992).
[28] M. Žnidarič, Phys. Rev. Lett. **106**, 220601 (2011).
[29] T. Prosen, Phys. Rev. Lett. **106**, 217206 (2011).