Nonequilibrium dynamical cluster theory

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Effect of spatially nonlocal correlations on the nonequilibrium dynamics of interacting fermions is studied by using the nonequilibrium dynamical cluster theory, a cluster generalization of the nonequilibrium dynamical mean-field theory (DMFT). The formalism is applied to interaction quenches in the Hubbard model in one and two dimensions, where the result is compared with those in the single-site DMFT, the time-dependent density matrix renormalization group (DMRG), and lattice perturbation theory. Both in one and two dimensions the double occupancy quickly thermalizes while the momentum distribution relaxes only on much longer time scales. For a two-dimensional square lattice we observe a strongly momentum-dependent evolution of the momentum distribution around the Fermi energy, where the relaxation is much faster near the momenta (0, π) and (π, 0) than near (π/2, π/2). The result is then interpreted as reflecting the momentum-anisotropic quasiparticle lifetime of the marginal Fermi liquid.

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Introduction. Simulating nonequilibrium dynamics of microscopic models for quantum many-body systems is a great challenge in theoretical physics [1], which may provide new insights into the role of strong correlations in high-temperature superconductors and other correlated systems by disentangling complex fluctuations along the real-time axis. So far, various approaches have been proposed. One focus has been on one-dimensional systems, for which the time-dependent density matrix renormalization group (DMRG) [2–4] and its variants have provided accurate simulations of the real-time evolution. Another approach comes from the opposite limit of infinite dimensions [5], where the nonequilibrium dynamical mean-field theory (DMFT) [6–9], that incorporates temporal fluctuations but approximates the self-energy as a spatially local function, becomes an exact scheme. However, the nonequilibrium properties of quantum systems in two dimensions, which lies in between these two extremes, remain far from being theoretically understood.

From an experimental point of view, too, the dynamics of two-dimensional (2D) quantum systems is of particular interest. A recent realization of the time-resolved angle-resolved photoemission spectroscopy (ARPES) begins to reveal temporal evolutions of the occupation n(k, ω, t) for correlated electrons in layered compounds [10–14]. For example, it has been shown that the quasiparticle recombination in the d-wave superconductor Bi2Sr2CaCu2O8+d occurs faster away from the “nodal line” (kx = ±kF) in the Brillouin zone than near the nodal line [14]. This kind of momentum-dependent relaxation dynamics can be related to nonlocal quantum correlations, which should become essential in low-dimensional quantum systems. We can then pose questions: What role do nonlocal correlations play in low-dimensional correlated systems out of equilibrium? And how can we take account of these effects systematically in real-time simulations?

These have motivated us in this Letter to present a new theoretical approach, namely the nonequilibrium dynamical cluster theory, which is the cluster extension of the nonequilibrium DMFT, or the nonequilibrium generalization of dynamical cluster theories [15]. In the DMFT formulation, we map a lattice model to a single-site impurity embedded in a dynamical mean field with the assumption of a local self-energy, which neglects nonlocal dynamical fluctuations. In cluster formalisms, this restriction is overcome by mapping the system onto a finite-size cluster problem with a spatially correlated dynamical mean field.

We then apply it to the interaction-quench problem in the Hubbard model in 1D and 2D, where we change the strength of the interaction abruptly in time. In cold atoms, where effective interactions can be tuned with Feshbach resonance or by changing the depth of optical lattice potentials, quantum quenches have become a standard procedure to trigger nonequilibrium dynamics [16–19], and the problem has attracted broad theoretical interests [20–29]. A naive expectation is that after the quench the system is highly excited and is characterized by a high effective temperature, so that the nonlocal correlations might be wiped out, as in equilibrium at high temperatures. However, we shall reveal that in 2D the momentum distribution, after experiencing prethermalization [22, 23, 30], exhibits a momentum-dependent relaxation dynamics: the distribution relaxes to the thermal one faster in the antinodal region [around (0, π) or (π, 0) in the Brillouin zone] than in the nodal region [around (π/2, π/2)]. The momentum-dependent relaxation, observed only when we go from the single-site to cluster formalism, comes from the nonlocal correlations. This observation is consistent with the quasiparticle lifetime of the marginal Fermi liquid, which is highly anisotropic in momentum space. We also examine a 1D system, with a comparison to exact DMRG result, to find rapid thermalization of the double occupancy similar to the 2D case apart from additional oscillations due to divergences at the band edges in the density of states.

Formulation. Let us formulate the nonequilibrium dynam-
ical cluster theory, by taking the Hubbard model as an example,

\[ H(t) = -J \sum_{\langle ij \rangle \sigma} (c_{i \sigma}^\dagger c_{j \sigma} + \text{h.c.}) - \mu \sum_{i \sigma} \hat{n}_{i \sigma} + U(t) \sum_{i} \hat{n}_{i \uparrow} \hat{n}_{i \downarrow}, \]

where \( c_{i \sigma}^\dagger \) creates a lattice fermion at \( i \)th site with spin \( \sigma \), \( \hat{n}_{i \sigma} = c_{i \sigma}^\dagger c_{i \sigma} \), \( J \) is the hopping amplitude, \( \mu \) is the chemical potential, \( U \) is the (time-dependent) interaction strength, and the sum \( \langle ij \rangle \) is taken over nearest-neighbor sites. There are two well-established constructions for the cluster mapping: the cellular DMFT [31,32] and the dynamical cluster approximant (DCA) [33,34]. Here we adopt DCA, since it preserves the periodicity of the lattice structure by construction.

The cluster reference system is defined by the action,

\[ S_{\text{clust}}[\Delta] = \int_{\mathcal{C}} \int_{\mathcal{C}} dt \int_{\mathcal{C}} dt' \sum_{i,j} d_{R_{i\sigma}}^\dagger(t) \Delta_{\sigma}(R_i; R_j; t, t') d_{R_{j\sigma}}(t') - \mu \int_{\mathcal{C}} \int_{\mathcal{C}} dt \sum_{i} \hat{n}_{R_{i\sigma}}(t) + \int_{\mathcal{C}} dt U(t) \sum_{i} \hat{n}_{R_{i\uparrow}}(t) \hat{n}_{R_{i\downarrow}}(t), \]

where \( d_{R_{i\sigma}}^\dagger \) creates a cluster fermion at a cluster site \( R_{i} \), \( \Delta_{\sigma}(R_i; R_j; t, t') \) is the hybridization function that will be determined self-consistently, \( \hat{n}_{R_{i\sigma}} = d_{R_{i\sigma}}^\dagger d_{R_{i\sigma}} \), and the time integral is taken along the Kadanoff-Baym contour \( \mathcal{C} \) [35] which runs as \( t = 0 \to t_{\text{max}} \to 0 \to -i\beta \) \( (t_{\text{max}}: \text{the maximum time up to which the system is evolved}, \beta: \text{the inverse temperature of the initial thermal state}) \). With this action, we define the cluster Green’s function \( G_{\sigma}^\text{clust}(R; R'; t, t') = -i(\langle \mathcal{C} d_{R_{i\sigma}}(t) d_{R_{i\sigma}}^\dagger(t') \rangle_{\text{clust}} \mathcal{C}) \), \( \mathcal{T} \) the contour-ordering operator along \( \mathcal{C} \) and \( (\cdots)_{\text{clust}} = \text{Tr}(\mathcal{T} e^{-iS_{\text{clust}}} \cdots)/\text{Tr}(\mathcal{T} e^{-iS_{\text{clust}}}) \).

If we denote by \( K \) the wave vector reciprocal to \( R \), we can write the Fourier-transformed cluster Green’s function as

\[ G_{\sigma}^\text{clust}(K; t, t') = \sum_{\mathcal{C}} e^{-iK \cdot R} G_{\sigma}^\text{clust}(R; R'; t, t'). \]

The Brillouin zone is divided into \( N_{c} \) sectors, each of which is centered at the corresponding \( K \). There are various choices of clusters. We adopt two cases, \( K_{x,y} = 2\pi n_{x,y}/N_{c} \) and \( K_{x,y} = (2n_{x,y} - 1)\pi/N_{c} \) \( (n_{x,y}: \text{integers}) \), and average the final results. In the lattice problem, an arbitrary wave vector \( k \) is represented as \( K + \mathbf{k} \), where \( \mathbf{k} \) spans from the center of the momentum sector to \( k \). The mapping from the lattice to the cluster problem (i.e., the choice of the hybridization function \( \Delta_{\sigma} \)) is defined such that the cluster Green’s function is reproduced by the lattice Green’s function averaged over the corresponding momentum sector,

\[ G_{\sigma}^\text{clust}[\Delta](K; t, t') = \frac{N_{c}}{N} \sum_{k} G_{\sigma}^\text{clust}(K + \mathbf{k}; t, t'), \]

with \( N \) the total number of \( k \) points. Green’s functions and self-energies are related via the cluster Dyson equation,

\[ (i\partial_{t} + \mu)G_{\sigma}^\text{clust}(K) - \Delta_{\sigma}(K) * G_{\sigma}^\text{clust}(K) - \Sigma_{\sigma}^\text{clust}(K) * G_{\sigma}^\text{clust}(K) = \delta_{\mathcal{C}}(t, t'), \]

and the lattice Dyson equation

\[ (i\partial_{t} + \mu)G_{\sigma}^\text{lat}(k) - \epsilon(k) * G_{\sigma}^\text{lat}(k) - \Sigma_{\sigma}^\text{lat}(k) * G_{\sigma}^\text{lat}(k) = \delta_{\mathcal{T}}(t, t'), \]

where \( \epsilon(k) = -2J \sum_{\langle ii \rangle} \cos k_{i} \) is the band dispersion, and \( \delta_{\mathcal{C}}(t, t') \) the contour delta function defined on \( \mathcal{C} \). In the nonequilibrium DCA, we identify the lattice self-energy with the cluster self-energy,

\[ \Sigma_{\sigma}^\text{clust}(K + \mathbf{k}; t, t') = \Sigma_{\sigma}^\text{clust}(K; t, t'), \]

that is, we neglect the \( \mathbf{k} \) dependence of \( \Sigma_{\sigma}^\text{clust}(K + \mathbf{k}; t, t') \). In this way, the problem is reduced to solving the cluster problem, for which one may use several possible solvers developed for the nonequilibrium DMFT, e.g., the weak-coupling perturbation theory [36,37], the noncrossing approximation (NCA) [38], and exact-diagonalization-based approaches [39,40].

In the present formalism, spatial correlations are systematically included within a finite range cutoff \( L = N_{C}^{1/d} \). In the large cluster-size limit \( (N_{c} \to \infty) \), the formalism should become exact in arbitrary dimensions. A virtue of the nonequilibrium DCA is that it provides a self-consistency scheme that updates the “noninteracting part” \( (\Delta_{\sigma}) \) of the action, so that it can describe “thermalization” in the long-time limit. This contrasts to other existing approaches for nonlocal correlations in the time evolution. For instance, the conventional lattice perturbation technique expands the self-energy with the noninteracting lattice Green’s function, so that the memory of the initial state is kept permanently. The cluster perturbation theory [41-43] decomposes the system into clusters, and treats the inter-cluster connections perturbatively, where the feedback to the exactly solved subsystems is limited. The dual-fermion approach provides another path to extend the DMFT, but its application to nonequilibrium situations is so far limited to a small-cluster and impurity problem [44,45]. Very recently, the equation-of-motion method has been applied to the 2D Hubbard model [29].

In the following, we study the interaction quench \( U(t) = 0 \to U > 0 \) for the Hubbard model, starting from the noninteracting zero-temperature state. We concentrate on the weak-coupling regime at half-filling, for which we employ the iterative perturbation theory (IPT) as a cluster solver with

\[ \Sigma_{\sigma}^\text{clust}(R; t, t') = U(t)U(t')G_{\sigma,0}(R; t, t')G_{\sigma,0}(-R; t', t)G_{\sigma,0}(R; t, t'). \]

Here \( G_{\sigma,0}(R; t, t') \) is the cluster Weiss mean-field propagator defined by

\[ (i\partial_{t} + \mu)G_{\sigma,0}(K) - \Delta_{\sigma}(K) * G_{\sigma,0}(K) = \delta_{\mathcal{T}}(t, t'). \]

We note that IPT works successfully for \( U \) smaller than or equal to half the bandwidth as an impurity solver in nonequilibrium DMFT calculations [37].

We have also obtained the result of the time-dependent DMRG [2-4] to benchmark the DCA result for the 1D system. By using a matrix-product state formalism in the thermodynamic limit [45], we can get rid of finite size effects,
observe that DCA nonlocality of the quantity. If we increase agreement is already seen at

\[ N = 1024 \]

for the methods other than DMRG. Compared to the infinite-coordination Bethe lattice where \( d(t) \) relaxes rapidly \([23]\), DMFT predicts a damped oscillation in \( d(t) \) for 1D lattice. As we proceed to DCA with \( N_c \geq 4 \) where the momentum space near the Fermi energy and the band edge can be distinguished, the oscillations are more pronounced. This suggests that the oscillation originates from the divergence of the density of states at the band edges in 1D. In fact, the oscillation period is roughly \( 2\pi / (4J) \) (4J is the bandwidth of 1D lattice). The DCA results quickly approach the exact DMRG (a fair agreement is already seen at \( N_c = 4 \)).

Unlike the double occupancy, \( \Delta n \) in DCA [Fig. 1(b)] does not converge so well against \( N_c \). This can be related to the nonlocality of the quantity. If we increase \( N_c \) up to 64, we observe that DCA+IPT approaches \( \Sigma^{(2)} \) for the 1D case. The deviation from DMRG must be attributed to quantum corrections from higher-order diagrams neglected in IPT. According to DMFT, \( \Delta n(t) \) exhibits a prethermalization plateau \([23]\) after a rapid initial drop, which is a characteristic feature of prethermalization \([22,51]\). According to DCA and DMRG, however, a clear prethermalization plateau is not observed. Instead, similar to \( d(t) \), we see an oscillation in \( \Delta n(t) \) which does not damp fast unlike in higher-dimension cases. The momentum distribution relaxes much slower than \( d(t) \), and is still far from the thermal distribution with \( \Delta n = 0 \) on the computationally accessible time scale.

While one might think that the 1D Hubbard model, being integrable \([52]\), should have a hindered thermalization, we find that the double occupancy takes, fairly soon after the quench, a value close to the thermal value [an arrow in Fig. 1(a)]. For integrable models, nonequilibrium states are often described by the generalized Gibbs ensemble \([53]\) using a macroscopic number of integrals of motion. Our analysis suggests that \( d(t) \) is not much sensitive to the non-trivial conserved quantities of the Hubbard model \([54]\), and the total energy together with the total number of particles almost fully describe the stationary value of \( d(t) \).

Next, we turn to the interaction quench for the 2D Hubbard model, where a point of interest is whether we have a qualitative change in going from 1D over to 2D. In Fig. 2 we plot the time evolution for \( d(t) \) and \( \Delta n(t) \) for 2D. We can see that \( d(t) \) quickly relaxes to the thermal value [an arrow in Fig. 2(a)] without generating long-lived oscillations. This is similar to the infinite dimensional case. For \( d(t) \), we find that the dependence on \( N_c \) is quite small (with DMFT already providing a good estimate), which implies that the nonlocal correlations are less relevant for local quantities in 2D.
If we turn to $\Delta n(t)$, which is a nonlocal quantity, we immediately notice that $\Delta n(t)$ now depends prominently on the position on the Fermi surface [while DMFT only gives a momentum-independent $\Delta n(t)$]. In the plot we have focused on the nodal ($\pi/2, \pi/2)$ and antinodal ($\pi, 0$) points, and we consider clusters up to $N_c = 16 \times 16$ (since we need $N_c \geq 4 \times 4$ to distinguish the nodal and antinodal sectors). As was the case in 1D, $\Delta n(t)$ is sensitive to $N_c$, and even with clusters as large as $N_c = 16 \times 16$ we still have a finite cluster-size effect. It seems that DCA+IPT is approaching $\Sigma^{(2)}$ in the large $N_c$ limit (at least for $\Delta n$) in this interaction regime. At present, going to larger clusters is technically difficult due to memory storage, since we have to keep $N/N_c$ large enough (in Fig. 2 we take $N = 256 \times 256$).

If we look more closely at Fig. 2(b), $\Delta n(t)$ evolves completely uniformly throughout the momentum space in the early stage ($tJ \lesssim 0.5$). After that, $\Delta n(t)$ suddenly starts to depend on momentum. The antinodal point ($\pi, 0$) relaxes faster than the nodal point ($\pi/2, \pi/2$), where a slowly damped oscillation appears in the time evolution. The latter is reminiscent of the 1D results. The DCA simulation suggests that the momentum distribution eventually reaches the thermal distribution with $\Delta n = 0$. If one goes to larger $U$, the momentum variation of $\Delta n(t)$ is weakened.

Now, let us examine what the momentum-dependent relaxation seen in $\Delta n(t)$ implies, based on the quasiparticle picture, which is valid in the weak-interacting regime. The lifetime $\gamma(k)$ of the quasiparticle with energy $\omega$ can be evaluated from the equilibrium retarded self-energy $\Sigma^{(2)}$.

$$\tau(k)^{-1} \propto \text{Im} \Sigma^{R}(k, \omega).$$

The 2D Hubbard model on the square lattice at half filling is special, since the one-particle dispersion has a van Hove singularity right at the Fermi energy $\epsilon_F$. This makes the density of states diverging logarithmically, and the system behaves as a “marginal Fermi liquid”, i.e., $\text{Im} \Sigma^{R}(k, \omega) \propto \omega$ around $\omega = \epsilon_F$ [56]. In the left panel of Fig. 3 we display $\text{Im} \Sigma^{R}(k, \omega)$ obtained from $\Sigma^{(2)}$. Even in the weak-coupling regime, $\text{Im} \Sigma^{R}(k, \omega)$ is highly anisotropic in momentum space: it is peaked at $(\pi, 0)$, while $(\pi/2, \pi/2)$ is a saddle point. In the right panel of Fig. 3 we compare the inverse quasiparticle lifetime $\text{Im} \Sigma^{R}(k, \omega)$ with the relaxation rate $\gamma$ for $\Delta n$. The latter is evaluated by fitting the DCA result for $\Delta n(t)$ [Fig. 2(b)] with a single exponential $Ae^{-\gamma t}$. We find the momentum dependence of $\gamma$ (with the qualitative tendency independent of $N_c$) is well reproduced by $\text{Im} \Sigma^{R}(k, \omega)$. This suggests that the momentum-dependent relaxation of $\Delta n(t)$ is in fact governed by the quasiparticles, which have a longer lifetime at $(\pi/2, \pi/2)$.

Summary. We have first formulated the nonequilibrium dynamical cluster theory to investigate the effect of nonlocal spatial correlations on nonequilibrium many-body systems by systematically changing the cluster size. We then applied the method to the interaction-quench problem for the Hubbard model in one and two dimensions, and found a peculiar momentum-dependent relaxation of quasiparticles in 2D. This may open an interesting avenue for probing marginal Fermi liquids in nonequilibrium. On the methodology, we found in the benchmark for 1D a good convergence for local properties, while the accuracy of non-local quantities is limited due to our perturbative solution of the impurity problem. Therefore, it will be important to test the cluster approach also using alternative nonequilibrium impurity solvers, such as NCA in the strong coupling regime [53], or Monte Carlo solvers on smaller clusters in the weak-coupling regime [52]. An interesting prospective application of the cluster method combined with weak-coupling perturbation theory is the simulation of the real-time dynamics of systems with long-range order (e.g. $d$-wave superconductivity or charge density waves), which is inaccessible by lattice perturbation theory.

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