Supplementary Material for "Exact Out-of-Time-Ordered Correlation Functions for an Interacting Lattice Fermion Model"

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I. EQUIVALENCE OF THE LOCAL AND LATTICE SUSCEPTIBILITIES AT GENERAL MOMENTUM

In this section, we explicitly show that the local dynamical charge susceptibility (8) of the Falicov-Kimball (FK) model, calculated from Eq. (7), is equal to the previously known result for the lattice dynamical charge susceptibility at general momentum [1, 2].

To see this, we substitute Eq. (7) in Eq. (8) to obtain

$$\chi(t,t') = i\theta(t-t') \sum_\alpha w_\alpha [R_\alpha^>(t,t')R_\alpha^<(t',t) - R_\alpha^<(t,t')R_\alpha^>(t',t)]. \tag{S.1}$$

We replace the greater Green's functions with the lesser, retarded, and advanced components by using the relations

$$\theta(t-t')R_\alpha^>(t,t') = \theta(t-t')R_\alpha^<(t,t') + R_\alpha^R(t,t'), \tag{S.2}$$

$$\theta(t-t')R_\alpha^>(t',t) = \theta(t-t')R_\alpha^<(t',t) - R_\alpha^A(t',t). \tag{S.3}$$

This results in the expression

$$\chi(t,t') = i \sum_\alpha w_\alpha [R_\alpha^R(t,t')R_\alpha^<(t',t) + R_\alpha^<(t,t')R_\alpha^A(t',t)], \tag{S.4}$$

or, in the Fourier transformed form,

$$\chi(\omega) = i \int \frac{d\omega'}{2\pi} \sum_\alpha w_\alpha [R_\alpha^R(\omega+\omega')R_\alpha^<(\omega') + R_\alpha^<(\omega+\omega')R_\alpha^A(\omega')]. \tag{S.5}$$

By means of the fluctuation-dissipation relation $R_\alpha^<(\omega) = f(\omega)[R_\alpha^A(\omega) - R_\alpha^R(\omega)]$ [$f(\omega) = 1/(e^{\beta\omega}+1)$ is the Fermi distribution function], Eq. (S.5) can be written as

$$\begin{aligned}\chi(\omega) = -i \int \frac{d\omega'}{2\pi} \sum_\alpha w_\alpha \Big\{ & f(\omega')R_\alpha^R(\omega+\omega')R_\alpha^R(\omega') \\ & - f(\omega+\omega')R_\alpha^A(\omega+\omega')R_\alpha^A(\omega') \\ & - [f(\omega') - f(\omega+\omega')]R_\alpha^R(\omega+\omega')R_\alpha^A(\omega') \Big\}.\end{aligned} \tag{S.6}$$

Let us recall that the configuration-dependent Green's function $R_\alpha(t,t')$ is in a nontrivial way related to the local Green's function and the self-energy [1],

$$\frac{1}{G^X(\omega)G^Y(\omega')} - \frac{1}{\sum_\alpha w_\alpha R_\alpha^X(\omega)R_\alpha^Y(\omega')} = \frac{\Sigma^X(\omega) - \Sigma^Y(\omega')}{G^X(\omega) - G^Y(\omega')}, \tag{S.7}$$

where $X, Y = R, A$. The right-hand side of Eq. (S.7) is the irreducible dynamical charge vertex function. The relation (S.7) can be proven as follows:

$$\begin{aligned}\sum_\alpha w_\alpha R_\alpha^X(\omega)R_\alpha^Y(\omega') &= \sum_\alpha w_\alpha \frac{R_\alpha^X(\omega) - R_\alpha^Y(\omega')}{R_\alpha^{Y-1}(\omega') - R_\alpha^{X-1}(\omega)} \\ &= \frac{\sum_\alpha w_\alpha [R_\alpha^X(\omega) - R_\alpha^Y(\omega')]}{R_0^{Y-1}(\omega') - R_0^{X-1}(\omega)} \\ &= \frac{G^X(\omega) - G^Y(\omega')}{[G^{Y-1}(\omega') + \Sigma^Y(\omega')] - [G^{X-1}(\omega) + \Sigma^X(\omega)]}.\end{aligned} \tag{S.8}$$

In deriving the second equality, we used $R_1^{X-1}(\omega) = R_0^{X-1}(\omega) - U$. In deriving the last equality, we used the impurity solution (4) and the impurity Dyson equation $G^X(\omega) = [R_0^{X-1}(\omega) - \Sigma^X(\omega)]^{-1}$ [note that $R_0^X(\omega)$ is the Weiss Green's function]. One immediately gets Eq. (S.7) from the last line of Eq. (S.8). Substituting Eq. (S.7) into Eq. (S.6), we arrive at

$$\begin{aligned}\chi(\omega) = -i \int \frac{d\omega'}{2\pi} \Bigg\{ & f(\omega') \frac{G^R(\omega+\omega')G^R(\omega')}{1 - G^R(\omega+\omega')G^R(\omega') \frac{\Sigma^R(\omega+\omega') - \Sigma^R(\omega')}{G^R(\omega+\omega') - G^R(\omega')}} \\ & - f(\omega+\omega') \frac{G^A(\omega+\omega')G^A(\omega')}{1 - G^A(\omega+\omega')G^A(\omega') \frac{\Sigma^A(\omega+\omega') - \Sigma^A(\omega')}{G^A(\omega+\omega') - G^A(\omega')}} \\ & - [f(\omega') - f(\omega+\omega')] \frac{G^R(\omega+\omega')G^A(\omega')}{1 - G^R(\omega+\omega')G^A(\omega') \frac{\Sigma^R(\omega+\omega') - \Sigma^A(\omega')}{G^R(\omega+\omega') - G^A(\omega')}} \Bigg\}.\end{aligned} \tag{S.9}$$

This is nothing but the lattice dynamical charge susceptibility of the FK model at general momentum [1, 2] [for the hypercubic lattice the general momentum corresponds to $X(\boldsymbol{q}) = \lim_{d\to\infty} \sum_{i=1}^d \cos q_i/d = 0$ [2, 3]]. The difference of the sign is due to the different definitions of the charge susceptibility. The physical reason for the coincidence between the local and lattice susceptibilities is explained in the main text.

II. LONG-TIME ASYMPTOTIC BEHAVIOR OF THE OUT-OF-TIME-ORDERED CORRELATION FUNCTION

In this section, we explain the long-time asymptotic form of the out-of-time-ordered correlation function $C(t) = -\langle [n^c(t), n^c(0)]^2 \rangle$ for the FK model.

Here $C(t)$ is determined from Eqs. (9), (10), and (11) in the main text. We note that $C(t)$ is obtained as a sum of products of $R_\alpha(t,t')$. Since $R_\alpha(t,t')$ is a 2-point function, any $R_\alpha(t,t')$ with $t,t' \in \tilde{\mathcal{C}}$ reduces to $R_\alpha(t,t')$ with $t,t' \in \mathcal{C}$. For example,

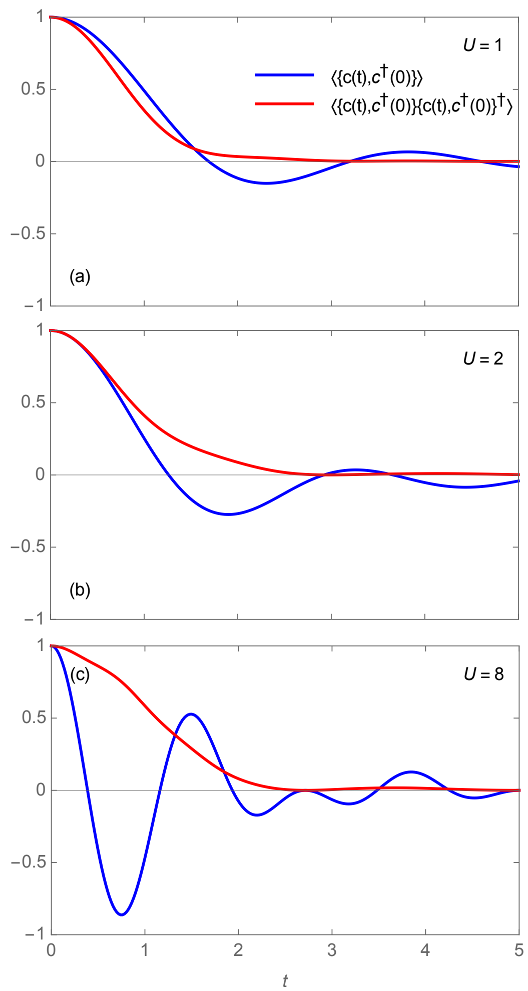

FIG. 1. Comparison between the retarded Green's function ($\times i$) $\langle\{c(t), c^\dagger(0)\}\rangle$ (blue curves) and the out-of-time-ordered correlation function $\langle\{c(t), c^\dagger(0)\}\{c(t), c^\dagger(0)\}^\dagger\rangle$ (red) for the FK model with $U = 1$ (a), $U = 2$ (b), and $U = 8$ (c). These functions do not depend on temperature.

$R_\alpha(t_+, 0_c) = R^>_\alpha(t, 0)$ and $R_\alpha(t_-, 0_c) = R^<_\alpha(t, 0)$. Thus $C(t)$ can be expressed as a contour function defined on the conventional Kadanoff-Baym contour $\mathcal{C}$. The result is

$$C(t) = \sum_\alpha w_\alpha |R^R_\alpha(t,0)|^2 \Big[|R^>_\alpha(t,0)|^2 + |R^<_\alpha(t,0)|^2 - |R^R_\alpha(t,0)|^2 + 2R^<_\alpha(t,t)R^<_\alpha(0,0) - iR^<_\alpha(t,t) - iR^<_\alpha(0,0) \Big]. \qquad \text{(S.10)}$$

The long-time behavior of $|R^{R,\gtrless}_\alpha(t,0)|$ is determined by the branch points in $R^{R,\gtrless}_\alpha(\omega)$ at the spectral edges ($\omega = \omega_c$), i.e., $R^{R,\gtrless}_\alpha(\omega) \sim (\text{regular part}) + (\text{const.}) \times \sqrt{\omega^2 - \omega_c^2}$ ($\omega \sim \omega_c$). By the saddle point approximation, one finds that $|R^{R,\gtrless}_\alpha(t,0)| \sim t^{-3/2}$ in the long-time limit both in the metallic and insulating phases (although the number of branch points changes at the phase transition point). This is also confirmed numerically. [If one takes a lattice other than the Bethe lattice, the asymptotic behavior may change according to the form of $R^{R,\gtrless}_\alpha(\omega)$ at the spectral edges.]

Since $R^<_\alpha(t,t)$ approaches a constant for $t \to \infty$, the long-time behavior of $C(t)$ is governed by $|R^R_\alpha(t,0)|^2 \sim t^{-3}$. The terms in the fourth power of R_α in Eq. (S.10) give subleading contributions to the long-time behavior.

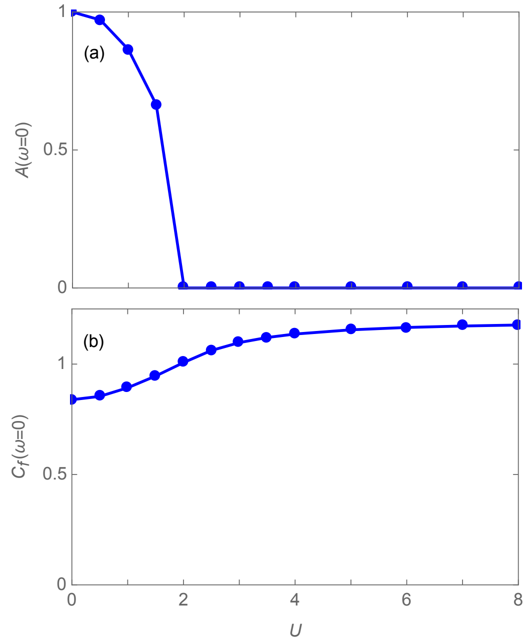

FIG. 2. Single-particle [$A(\omega)$ (a)] and OTOC [$C_f(\omega)$ (b)] spectral functions for the FK model at zero frequency. These functions do not depend on temperature.

III. FERMIONIC OUT-OF-TIME-ORDERED CORRELATION FUNCTION

In this section, we show the results for the out-of-time-ordered correlation function constructed from the fermionic operators $V = c_i^\dagger, W = c_i$. A natural extension of the definition of the OTOC (1) to fermionic operators is given by $\langle\{W(t), V(0)\}\{W(t), V(0)\}^\dagger\rangle$, where we have replaced the commutator in Eq. (1) with an anticommutator. This fermionic OTOC can be evaluated exactly for the infinite-dimensional FK model with the same technique as explained in the main text:

$$\begin{aligned} C_f(t) &\equiv \langle\{c(t), c^\dagger(0)\}\langle\{c(t), c^\dagger(0)\}^\dagger\rangle \\ &= \sum_\alpha w_\alpha [R^>_\alpha(t,0) - R^<_\alpha(t,0)][R^<_\alpha(0,t) - R^>_\alpha(0,t)] \\ &= \sum_\alpha w_\alpha |R^R_\alpha(t,0)|^2. \end{aligned} \qquad \text{(S.11)}$$

It satisfies $C_f(t) \geq 0$.

In Fig. 1, we compare the retarded Green's function $iG^R(t,0)$ and $C_f(t)$ for several U. We note that both $G^R(t,0)$

and $C_f(t)$ are independent of the system's temperature, since the retarded components of Green's functions and the self-energy form a closed set of self-consistent equations in the case of the FK model, and can be determined independently of the Matsubara components. As one can see in Fig. 1, the timescale on which $C_f(t)$ changes is comparable to that of $G^R(t,0)$ (and the dynamical charge correlation function). The initial drop of $C_f(t)$ is delayed compared with $G^R(t,0)$ in the insulating phase ($U \geq 2$). In the long-time limit, the functions decay as power laws: $iG^R(t,0) \sim t^{-3/2}$ and $C_f(t) \sim t^{-3}$.

To illustrate the dependence of the OTOC $C_f(t)$ on the interaction U, we define the OTOC spectral function

$$C_f(\omega) = \int_0^\infty dt\, e^{i\omega t} C_f(t). \tag{S.12}$$

In Fig. 2, we compare $C_f(\omega)$ at $\omega = 0$ with the single-particle spectral function $A(\omega) = -\frac{1}{\pi}\mathrm{Im}G^R(\omega)$ at $\omega = 0$ for the FK model. In the metallic phase ($U < 2$), there is a nonzero spectral weight at the Fermi energy, while in the insulating phase ($U > 2$) the energy gap opens and the spectral weight vanishes. On the other hand, $C_f(\omega = 0)$ grows as U is increased, and saturates in the strong-coupling limit. This implies that in the insulating phase, even though the single-particle motions are frozen at low energy, the information spreading still occurs to some extent.

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[2] J. K. Freericks and V. Zlatić, Rev. Mod. Phys. **75**, 1333 (2003).
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