Violation and revival of Kramers’ degeneracy in open quantum systems

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Kramers’ theorem ensures double degeneracy in the energy spectrum of a time-reversal symmetric fermionic system with half-integer total spin. Here, we are trying to go beyond the closed system and discuss Kramers’ degeneracy in open systems out of equilibrium. A natural way to extend the Kramers’ degeneracy in open quantum systems is by the degeneracy of different spins’ spectra together with the vanishing interspin spectrum. We find the violation of Kramers’ degeneracy in time-reversal symmetric open quantum systems is locked with whether the system reaches thermal equilibrium. After a general coupling to an environment in a time-reversal symmetry-preserving way, the Kramers doublet experiences an energy splitting at a short time and then a recovery process. We verified the violation and revival of Kramers’ degeneracy in a concrete model of interacting fermions and we find Kramers’ degeneracy is restored after the local thermalization time. By contrast, for time-reversal symmetry \(T\) with \(T^2 = 1\), we find that although there is a violation and revival of spectral degeneracy for different spins, the inter-spin spectral function is always nonzero. We also prove that the Kramers’ degeneracy in spectral function protected by unitary symmetry can always be maintained.

Introduction. Kramers’ degeneracy theorem tells us for fermionic systems with half-integer total spin where time-reversal symmetry (TRS) is presented, all energy levels are doubly degenerate \[1,2\]. This theorem plays a vital role in the quantum-spin Hall effect \[3,4\] as well as in the stability of the superconducting phase with disorder \[5\]. Kramers’ theorem is expected for thermal equilibrium systems since the grand canonical distribution is only related to the Hamiltonian where the double degeneracy is presented. This can be proved straightforwardly in equilibrium systems \[6\]. Recently, topological states protected by TRS in non-Hermitian systems and Floquet systems are widely discussed in varieties of systems \[7–11\]. However, we must be cautious because anti-unitary symmetry in effective Hamiltonian is fragile in open quantum systems. A later discovery made by McGinley and Cooper says that TRS is only a good symmetry in equilibrium systems \[6\]. In this work, we go beyond the perturbation theory and study the whole dynamical process, focusing on the Kramers’ degeneracy for a time-reversal invariant (TRI) interacting fermion system with a TRS preserving interaction between the system and the bath. We find that the Kramers’ degeneracy is locked with thermal equilibrium. We find a violation of Kramers’ degeneracy after a sudden coupling to an environment, and the violation enlarges with time while it shrinks afterward as is shown in Fig. 1. The Kramers’ degeneracy revives as the system gradually reaches new thermal equilibrium. Due to the connection between Kramers’ degeneracy and local thermalization, we also find the Kramers’ degeneracy in the spectrum can experience a violation and revival process in isolated systems that satisfy the eigenstate thermalization hypothesis (ETH).

In the following, we first establish a general relation between Kramers’ degeneracy and single-particle spectral functions. Then with the help of solvable interacting models, we can calculate the quench dynamics of the spectral function and the distribution function with a sudden coupling to a bath. By checking the time scale of distribution function reaching thermal equilibrium and Kramers’ degeneracy signal in spectral functions, we can draw our conclusion. We also discussed how spectral functions evolve for system-to-bath interaction baring TRS \(\tilde{T}\) with \(\tilde{T}^2 = 1\) and unitary symmetry \(S\) as a comparison. We stress that our conclusion applies to general interacting fermion systems and is not restricted by the Markovian approximation. By this study, we find Kramers’ degeneracy only emerges in thermal equilibrium systems, which implies TRS is only a good symmetry in equilibrium systems and the breaking extent of Kramers’ degeneracy can

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be set as a measure of the extent of the system being away from equilibrium.

General Theory. We consider a quantum many-body system with spin-1/2 fermions $\hat{c}_{j,\sigma}$, where $\sigma = \pm$ labels spin states, and $j$ is the mode index. Under the time-reversal transformation, the fermionic annihilation operator $\hat{c}_{j,\sigma}$ satisfies $\hat{T}\hat{c}_{j,\sigma}\hat{T}^{-1} = \sigma\hat{c}_{j,-\sigma}$ and thus $\hat{T}^2 = (-1)^N$. Here $N_i$ is the fermion number in the system. We prepare the system in thermal equilibrium of initial Hamiltonian $\hat{H}_i$ as $\hat{\rho}_0 = e^{-\beta\hat{H}_i}/Z$, with $Z = \text{tr}[e^{-\beta\hat{H}_i}]$. We assume $\hat{H}_i$ is the system Hamiltonian with TRS satisfying $\hat{T}\hat{H}_i\hat{T}^{-1} = \hat{H}_i$. Kramers’ theorem states that the eigenstate of $\hat{H}_i$ with odd $N_i$ should have a pairwise degeneracy [17]: Given any eigenstate $|\psi_i\rangle$, satisfying $\hat{H}_i|\psi_i\rangle = E_i|\psi_i\rangle$, one can show that for $|\psi_2\rangle = \hat{T}|\psi_1\rangle$, it satisfies $\hat{H}_i|\psi_2\rangle = E_2|\psi_2\rangle$ and $\langle\psi_1|\psi_2\rangle = 0$. As a comparison, $\hat{H}_i|\psi_2\rangle = E_0|\psi_2\rangle$, without $\langle\psi_1|\psi_2\rangle = 0$, also works in the even $N_i$ subspace and is not sufficient for proving the existence of the degeneracy.

However, for general interacting quantum systems, it is hard to prove a specific eigenstate experimentally. It is Green’s function of local operators that can be measured by various experimental protocols [18], which in general give the spectrum and distribution function information of the quasi-particles. Here we are trying to discuss the Kramers’ degeneracy in open quantum systems, where even no eigenstates of the system are well defined. Therefore we have to introduce Green’s function form of the Kramers’ degeneracy. First, we introduce real-time Green functions $G^\sigma_{\alpha\sigma}(t',t)$, which are defined as

$$iG^\sigma_{\alpha\sigma}(t',t) = \text{tr}[\hat{\rho}_0\hat{c}_{j,\sigma}(t)\hat{c}^\dagger_{j,\sigma}(t')],$$

$$-iG^\sigma_{\alpha\sigma}(t,t') = \text{tr}[\hat{\rho}_0\hat{c}^\dagger_{j,\sigma}(t)\hat{c}_{j,\sigma}(t')],$$

where $\hat{c}_{j,\sigma}(t) = e^{i\hat{H}_i t}\hat{c}_{j,\sigma}e^{-i\hat{H}_i t}$ is fermion annihilation operator in Heisenberg picture. Here $tr$ is over the Hilbert space of the system. Then it is straightforward to show that there is an analogy of the Kramers’ theorem $G^{++}_{\alpha\alpha}(t,t') = G^{--}_{\alpha\alpha}(t,t') = 0$ in thermal equilibrium [6]. Here, $G^{\pm\pm}_{\alpha\alpha}(t,t') = G^{\pm\pm}_{\alpha\alpha}(t',t) = 0$, as an analogy of $\langle\psi_1|\psi_2\rangle = 0$, is a signature of having $\hat{\mathcal{F}}^2 = (-1)^N$. Using their relation to the spectral function $\mathcal{A} = i(G^+-G^-)/2\pi$, we have $\mathcal{A}_{++} = \mathcal{A}_{--}$ and $\mathcal{A}_{+-} = \mathcal{A}_{-+} = 0$ in thermal equilibrium.

In this work, we are interested in understanding the Kramers’ degeneracy in the quench dynamics from the Green’s function perspective. At $t = 0$, we change the Hamiltonian from $\hat{H}_i$ to $\hat{H}_f$, which also satisfies $\hat{T}\hat{H}_f\hat{T}^{-1} = \hat{H}_f$. In particular, we couple the original system to an additional bath by taking $\hat{H}_f = \hat{H}_i + \hat{V}$, where $\hat{V} = \sum_j V_j\hat{O}_j\hat{c}_{j,\sigma}$, satisfying $\hat{T}\hat{O}_j\hat{T}^{-1} = \hat{O}_j$ and $\hat{T}\hat{c}_{j,\sigma}\hat{T}^{-1} = \hat{c}_{j,\sigma}$. Operators $\hat{O}_j$ are TRS operators in the system and the environment. Generally, using the time-reversal transformation, one can show that for $t, t' > 0$ we have

$$i(G^{++}_{\alpha\alpha} - G^{--}_{\alpha\alpha}) = \langle [\hat{O}_j,\hat{c}_{j,\sigma}(t')\hat{c}^\dagger_{j,\sigma}(t)]\hat{O}_j \rangle_B,$$

$$-2iG^{++}_{\alpha\alpha} = \langle [\hat{O}_j,\hat{c}_{j,\sigma}(t')\hat{c}^\dagger_{j,\sigma}(t)]\hat{O}_j \rangle_B.$$

Here $\Delta\hat{c}_{j,\sigma}(t,t') = \hat{O}_j(t)\hat{O}_j^\dagger(t') - \hat{O}_j^\dagger(t')\hat{O}_j(t)$ is the quantum expectation on the bath density matrix, which is assumed to be thermal with inverse temperature $\beta_B$. Since the bath contains a much larger degree of freedom, we assume that it does not evolve when coupled to the small system. Similar relations hold for $G^{0\sigma\sigma}$ and thus $\mathcal{A}_{\alpha\sigma}$.

In the short time limit, we have $\Delta\hat{c}_{j,\sigma}(t,t') \approx \hat{O}_j(t)\hat{O}_j^\dagger(t')\hat{O}_j(t)\hat{O}_j^\dagger(t') + \hat{O}_j^\dagger(t')\hat{O}_j(t)\hat{O}_j^\dagger(t')\hat{O}_j(t)$. The leading-order contribution is from $[\hat{H}_i,\hat{O}_j]\hat{\rho}_0$. Considering that $\hat{\rho}_0 = e^{-\beta_0\hat{H}_i}$, therefore $[\hat{H}_i,\hat{\rho}_0] = [\hat{V},\hat{\rho}_0] = \sum_j V_j\hat{c}_{j,\sigma}^\dagger\hat{O}_j\hat{c}_{j,\sigma}$, we can see, the TRS of $\hat{O}_j$ does not ensure $[\hat{O}_j,\hat{\rho}_0] = 0$, therefore in general $[\hat{H}_i,\hat{\rho}_0] \neq 0$. As a result, $G^{++}_{\alpha\alpha} \neq G^{+-}_{\alpha\alpha}, G^{\pm\pm}_{\alpha\alpha} \neq 0$ and the Kramers’ degeneracy is broken. This generalizes the previous analysis using Markovian baths [16]. As a comparison, for unitary symmetries interchanging + and −, one finds a similar relation for $i(G^{++}_{\alpha\alpha} - G^{--}_{\alpha\alpha})$, but with $\Delta\hat{c}_{j,\sigma}(t,t') = \hat{c}_{j,\sigma}(t') - \hat{c}_{j,\sigma}(t) = 0$. It means the degeneracy protected by unitary symmetry is stable in dynamical evolutions. We also notice that the condition $\Delta\hat{c}_{j,\sigma}(t,t') \neq 0$ is very general and has a more natural understanding than the extended Schur Lemma argument given previously [12].

On the other hand, for $t, t' \gg t_h$, where $t_h$ is the thermalization time, we expect the total system to thermalize and $\hat{\rho}_{\alpha\beta}(t) \approx \hat{\rho}_{\alpha\beta}(t) \approx e^{-\beta'(t)\hat{H}_B(t)/t\beta(t)}[\text{tr}[e^{-\beta(t)\hat{H}_B(t)/t\beta(t)}]]$ under simple probes. Here $\hat{H}_B$ is the Hamiltonian of the bath. Consequently, we find $G^{++}_{\alpha\alpha} = G^{--}_{\alpha\alpha}, G^{0\alpha\alpha} = 0$, and the Kramers’ degeneracy is restored. For a large system-bath coupling, the characteristic time scale $t_h$ resembles its counterpart in isolated quantum systems, where $t_h \sim \beta_0$ for strongly interacting models and $t_h \sim 1/\Gamma$ with quasi-particle decay rate $\Gamma$ for weakly interacting models [19-21].

Before turning to concrete examples, we add a few comments. First, the violation and revival of Kramers’ degeneracy also exists in isolated quantum systems that satisfy ETH, where $\hat{H}_i$ is different from $\hat{H}_i$ by certain parameters [22].
In this case, (2) still works, without the average over bath density matrix. In the long-time limit, although the fine-grained density matrix $\rho(t)$ may differ from the thermal density matrix since the unitary evolution preserves the total entropy, we expect local thermalization $\hat{\rho}(t) \sim \rho^{eq}$, $e^{-\beta H / \hbar}$ [22,23]. Here, $\sim$ means the equivalence under measurement of local operators. As a comparison, the violation can not be restored if the system is many-body localized.

Second, it is helpful to compare the above results with TRS with $\hat{S}^2 = 1$ or unitary symmetry $S$. We choose the single-particle transformation to be $\hat{T} = \sigma, K$ or $S = i\sigma_\tau$. Here $K$ is the complex conjugate operator. In both cases, the symmetry imposes $G_{++} = G_{--}$ in thermal equilibrium, while generally $G_{+-} \neq 0$. When coupled to the bath, for TRS $\hat{T}$, the $G_{++}$ firstly breaks and then gets restored. While for $S$, the $G_{++} = G_{--}$ is always preserved during the evolution.

Concrete Model. We consider the quench by coupling the system to an external bath at $t = 0$ (here we choose the quench as an example). Similar results hold if the coupling is turned on slowly [22], with system-bath coupling

$$H_{SB}(t) = \theta (t) \sum_{j,j',b_1 b_2} V_{j j', b_1 b_2} \left( \sum_{\tau \bar{\tau} \sigma} c_{j \tau \sigma} \tilde{h}^{\sigma}_{\bar{\tau} \sigma} c_{j' \bar{\tau} \sigma} \right) \psi_{b_1} \psi_{b_2}. $$

Here, to be concrete, we choose the bath to be an additional SYK model with $M \gg N$ fermion modes ($b_1, b_2 = 1, 2, \ldots, M$) [36–39]. This corresponds to

$$H_B = \sum_{j_1, j_2, b_1, b_2} J_{b_1 b_2}^R \psi_{b_1}^\dagger \psi_{b_2} / 4. $$

We further choose the distribution of $J_{b_1 b_2}$ to take similar form as (4), with $N$ replaced by $M$. Generalizations to other bath models are straightforward. The coupling strength satisfies

$$|V_{j_1 j_2 b_1 b_2}| = 0, \quad \left| |V_{j_1 j_2 b_1 b_2}|^2 \right| = V^2 / N M^2. $$

This guarantees that $H_{SB}$ does not affect the evolution of the bath [36–39], consistent with our previous assumption. We also choose the $\hat{h}$ to take general form

$$\hat{h} = \bar{\mu} I \otimes I + K_x \tau_x \otimes I + K_z \tau_z \otimes I$$

$$+ J_y \tau_y \otimes \sigma_x + J_y \tau_y \otimes \sigma_y + J_z \tau_y \otimes \sigma_z, $$

where $\bar{\mu}, K_x, K_z, J_{x,y,z}$ are independent parameters. The form of $\hat{h}$ ensures the ensemble of couplings are also invariant under the TRS $\hat{T}$. Here we have extended $\hat{T}$ to the full system by defining $\hat{T} \psi_j \hat{T}^{-1} = \psi_j$.

In the large-N limit, the Green’s functions $G^\sigma$ of SYK-like models satisfy the Schwinger-Dyson equation on the Keldysh contour, and the quench dynamics can be simulated by solving corresponding integral equations. Explicitly, we have

$$(i\hbar \partial_t - \hat{h}) \circ G^\sigma = \Sigma^R \circ G^\sigma + \Sigma^\omega \circ G^A, $$

where $\circ$ includes the convolution in real-time, as well as multiplication in $\sigma$ and $\tau$ space. The self-energy is given by melon diagrams shown in Fig. 2, which leads to

$$\Sigma^{\omega, \sigma, \sigma'}_{\tau, \tau'}(t, t') = J^2 \delta_{\sigma \sigma'} \delta_{\tau \tau'} G^{\omega, \sigma, \sigma'}_{\tau, \tau'}(t, t')$$

$$+ V^2 \chi^{\omega, \tau, \sigma, \sigma'}_{\sigma, \sigma'}(t, t') \theta(t) \theta(t'). $$

Here $\chi^{\omega, \tau, \sigma, \sigma'}(t, t') = G^{\omega, \tau, \sigma, \sigma'}(t, t')$ is the bath correlation function. The retarded/advanced Green’s functions are related to $G^\omega$ by $G^R(t_1, t_2) = \theta(t_2) (G^\omega(t_1, t_2) - G^\omega(t_2, t_1))$ and $G^A(t_1, t_2) = \theta(t_1) (G^\omega(t_1, t_2) - G^\omega(t_2, t_1))$. Similar relations hold for self-energies. Using these relations, (9) and (10) become closed. The numerical approach for solving (9) and (10) with discretized time has been well explained in previous works [37,40–42].

Numerical Results. We now present numerical results of the quench dynamics. Results for slow couplings and periodic couplings are given in Supplemental Material [22]. We choose $J_y = J_z = V = 1$, and arbitrarily chosen parameters in $\hat{h}$ and $\bar{\mu}$. Given the real-time Green’s function $G^\sigma(t, t')$, we define the
temporal Green’s function $\tilde{G}^\tau(t_r, t)$ at time $t$ by

$$\tilde{G}^\tau(t_r, t) \equiv \begin{cases} G^\tau(t + t_r, t) & t_r \leq 0, \\
G^\tau(t, t - t_r) & t_r > 0. \end{cases}$$

This definition preserves the causality of the unitary evolution. Here $G^\tau$ and $G^\hat{\tau}$ are in matrix form, and the sub-indices are omitted. We define the Fourier transform with respect to $t_r$.

The temporal spectral function $\mathcal{A}(\omega, t)$ then reads

$$\mathcal{A}(\omega, t) = \frac{i}{2\pi} \int dt_r e^{i\omega t_r} (\tilde{G}^\tau(t_r, t) - \tilde{G}^\hat{\tau}(t_r, t)).$$

In numerics, we focus on the first site with $\tau = +$ and drop the corresponding pseudospin indices for conciseness. The results for $\mathcal{A}_{++}(\omega, t)$, $\mathcal{A}_{--}(\omega, t)$, and $\text{Re} \mathcal{A}_{+-}(\omega, t)$ are shown in Fig. 3(a). Before the quench, the system is in thermal equilibrium and the Kramers’ theorem ensures $\mathcal{A}_{++}(\omega, 0) = \mathcal{A}_{--}(\omega, 0)$ and $\mathcal{A}_{+-}(\omega, 0) = 0$. After we couple the system to the bath ($t > 0$), the degeneracy is lifted. As an example, we find a large discrepancy between $\mathcal{A}_{++}$ and $\mathcal{A}_{--}$, as well as a non-vanishing $\mathcal{A}_{+-}$ at $t = 5$. When the time $t$ becomes longer, $\mathcal{A}_{++}$, $\mathcal{A}_{--}$, and $\mathcal{A}_{+-}$ decays, and becomes almost invisible at $t = 30$.

Our previous analysis shows the revival of Kramers’ degeneracy happens when the system arrives at equilibrium with the bath. In a quantum many-body system, the local thermalization can be diagnosed by quantum distribution function $F(\omega, t)$ at time $t$. It can then be defined as

$$F(\omega, t) \mathcal{A}(\omega, t) = \frac{i}{2\pi} \int dt_r e^{i\omega t_r} (\tilde{G}^\tau(t_r, t) + \tilde{G}^\hat{\tau}(t_r, t)).$$

In thermal equilibrium, we have $F(\omega) = 1 - 2n_F(\omega) = \tanh(\beta\omega/2)$, with Fermi-Dirac distribution function $n_F(\omega)$.

We plot $F(\omega, t)$ for different $t$ in Fig. 3(b). Shortly after the quench, $F(\omega, t)$ significantly deviates from the $\tanh(\beta\omega/2)$ and the system is far from equilibrium. At longer time $t = 15$, $F(\omega, t)$ approaches the $\tanh(\beta\omega/2)$, although there is still visible oscillations in low frequency. The system almost thermalizes at $t = 30$. The black dashed curve corresponds to a plot of $\tanh(\beta\omega/2)$. (c) The log-plot of $\Delta_1$, or $\Delta_2$, as a function of time $t$, which characterize the breaking of the Kramers’ degeneracy. The dashed lines correspond to the results of the linear fittings. As a comparison, we also plot the evolution of spectral $\mathcal{A}$ for a model [44] with symmetry $\tilde{T}(\tilde{T}^2 = 1)$ in (d) and (e).

FIG. 3. Numerical results for the TRI SYK model coupled to bath. We choose $\beta J = \beta J = 6, V = J$, and we set $\beta = 2\pi$ as the unit of time. We further set $(\mu, K, K, J, J, J_J,J_J) / J = (0, 0.1, 0.2, 0.3, 0.15, 0.2)$ and $(\mu, K, K, J, J, J_J,J_J) / J = (0, 0.4, 0.4, 0.6, 0.36, 0.2)$. (a). The spectral function $\mathcal{A}_{++}$, $\mathcal{A}_{--}$ and $\text{Re} \mathcal{A}_{+-}$ as a function of evolution time $t$. There is a breaking and restoring of Kramers’ degeneracy. (b). The quantum distribution $F(\omega)$ at different time $t$. The system almost thermalizes at $t = 30$. The black dashed curve corresponds to a plot of $\tanh(\beta\omega/2)$. (c) The log-plot of $\Delta_1$, or $\Delta_2$, as a function of time $t$, which characterize the breaking of the Kramers’ degeneracy. The dashed lines correspond to the results of the linear fittings. As a comparison, we also plot the evolution of spectral $\mathcal{A}$ for a model [44] with symmetry $\tilde{T}(\tilde{T}^2 = 1)$ in (d) and (e).
Kramers’ degeneracy experienced a breaking and restoring process. We further show it works for more general coupling schemes. We find the revival of Kramers’ degeneracy happens after the local thermalization time $t_{th}$. Similar results can be obtained for TRS $T$ with $T^2 = 1$. But distinctively, $A_{−}(ω) = 0$ is not satisfied at all the time. It also means $A_{++}(ω) = −A_{−−}(ω)$ alone cannot be seen as the condition for Kramers’ degeneracy. It is also verified that for systems where local thermalization is hard to establish, the violation of Kramers’ degeneracy will not recover.

Further, as we have seen, after coupling to a bath, although Kramers’ degeneracy can be recovered, there is always a large portion of time Kramers’ degeneracy is violated. For this reason, if we start from a pure state in Kramers’ space in the initial Hamiltonian, decoherence will happen and be maintained. The decoherence in the final state can be partially implied by the line shape change in the final state spectrum compared with the initial state spectrum. In this sense, we find different respects in TRS of open systems. If a physical result is more sensitive to phase coherence, such as the quantization of the conductance in topological insulators, we argue that these results cannot be protected by the revival of Kramers’ degeneracy [16]. On the other hand, like in superconductors, the pairing is more relevant to the energy degeneracy of the Kramers’ pair. Therefore the superconducting phenomenon may be more stable against the environment. Furthermore, as we see that equilibrium or not is very important for time-reversal symmetric systems, but many transport theories are based on linear response theory, which attributes transport properties as a manifestation of equilibrium correlations. We leave a careful study in these directions to future works.

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[22] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevB.105.L241106 for (1) the derivation of (2); (2) the violation and revival of Kramers’ degeneracy in isolated thermalized quantum systems; (3) the absence of revival in many-body localized quantum systems; and (4) the study of slow coupling and periodic coupling.


[44] We consider the model with $\tilde{T}$ by choosing
$$h = \mu I \otimes I + K_\tau \otimes I + J_\tau \otimes \sigma_i + J_i \tau_i \otimes \sigma_i + J_\tau \otimes \sigma_i$$
and
$$\tilde{h} = \mu I \otimes I + \tilde{K}_\tau \otimes I + \tilde{J}_\tau \otimes \sigma_i + \tilde{J}_i \tau_i \otimes \sigma_i + \tilde{J}_\tau \otimes \sigma_i.$$