

Generating function formula of heat transfer in harmonic networks

Keiji Saito^{1,2} and Abhishek Dhar³¹*Graduate School of Science, University of Tokyo, 113-0033, Japan*²*CREST, Japan Science and Technology (JST), Saitama, 332-0012, Japan*³*Raman Research Institute, Bangalore 560080, India*

(Received 6 December 2010; published 21 April 2011)

We consider heat transfer across an arbitrary classical harmonic network connected to two heat baths at different temperatures. The network has N positional degrees of freedom, of which N_L are connected to a bath at temperature T_L and N_R are connected to a bath at temperature T_R . We derive an exact formula for the cumulant generating function for heat transfer between the two baths. The formula is valid even for $N_L \neq N_R$ and satisfies the Gallavotti-Cohen fluctuation symmetry. Since harmonic crystals in three dimensions are known to exhibit different regimes of transport such as ballistic, anomalous, and diffusive, our result implies validity of the fluctuation theorem in all regimes. Our exact formula provides a powerful tool to study other properties of nonequilibrium current fluctuations.

DOI: [10.1103/PhysRevE.83.041121](https://doi.org/10.1103/PhysRevE.83.041121)

PACS number(s): 05.70.Ln, 05.40.-a, 44.10.+i, 63.22.-m

I. INTRODUCTION

Nonequilibrium systems typically generate currents of mass or energy. Understanding the general features of currents and their fluctuations is one of the main goals in nonequilibrium statistical physics. In this context the fluctuation theorem (FT) is a remarkable discovery [1,2]. This has been theoretically [1–4] and experimentally demonstrated [5] in many systems. These studies have pointed to the significance of the large deviation function (LDF) of the current and the related cumulant generating function (CGF) in understanding nonequilibrium steady states. Some other interesting related developments include the study of Bertini and co-workers [6], who introduced a hydrodynamic fluctuation theory to study large dynamic fluctuations in steady states, and that of Bodineau and Derrida [7,8], who conjectured an additivity principle for the LDF and CGF of current, from which one can predict the quantitative behavior of higher-order correlations of currents.

In the context of transport, most analytic results on LDFs and FTs are on systems where the bulk dynamics is stochastic, such as the simple exclusion process, zero range process, Brownian motors, etc. [3,8,9]. It is of general interest to consider and develop these arguments for systems with bulk Hamiltonian dynamics. However, exact analysis here is generally difficult. For example, even the problem of demonstrating Fourier's law of heat conduction in a deterministic system has proved to be difficult and has led to many surprises [10–12]. Heat conduction in harmonic lattices is one exception where many nonequilibrium properties can be precisely discussed. The average heat current, the main focus of work so far, is given by a Landauer-like formula in terms of phonon transmission coefficients [13]. Using the transport formula it was recently demonstrated [14] numerically that disordered harmonic crystals in two and three dimensions can exhibit different regimes of transport such as ballistic, localized, anomalous, and diffusive. Given that this simple deterministic model exhibits various regimes of transport, it is of interest to study the generic features of nonequilibrium current fluctuations in this system.

In this paper, we derive the general formula of the CGF for heat current in an arbitrary harmonic lattice connected to two heat baths, which provides a basis to explore generic features of current fluctuations. Consider heat transfer through a system from a bath at temperature T_L to a bath at temperature T_R . Let Q be the heat transferred from the left reservoir to the system during measurement time τ . In general, the distribution of heat $P(Q)$ has an asymptotic form $P(Q) \sim e^{\tau h(q)}$ at large τ where $h(q = Q/\tau)$ is the LDF. The CGF $\mu(\lambda)$ generates cumulants of the heat transferred and is defined through the relation $\langle e^{\lambda Q} \rangle \sim e^{\tau \mu(\lambda)}$. The LDF $h(q)$ and the CGF $\mu(\lambda)$ are connected through the Legendre transform $\mu(\lambda) = \max_q [\lambda q + h(q)]$. Properties of heat current fluctuations are contained in $h(q)$ or equivalently in $\mu(\lambda)$, and various results such as the steady state FT and the additivity principle conjecture can be stated in the framework of either the LDF or the CGF. For heat conduction, the steady-state FT of Gallavotti-Cohen (GC) [2] implies the symmetry relation $\mu(\lambda) = \mu(-\lambda - \Delta\beta)$, where $\Delta\beta = 1/T_R - 1/T_L$, and is referred to as the GC symmetry. There are examples where the symmetry of $\mu(\lambda)$ does not imply the FT [15]. However, the CGF and its symmetry property themselves provide important information on current fluctuations. Among these, one of the most interesting consequences of the symmetry relation is that it leads to the standard linear response results such as Onsager reciprocity and Green-Kubo relations [3,16] and in addition makes predictions of responses in the far-from-equilibrium regime [17–19]. So far, for Hamiltonian systems, the CGF has been analytically obtained for one- and two-particle systems [20,21] and for a one-dimensional quantum harmonic chain [22]. Here we obtain a general formula for the CGF of a harmonic system in terms of the transmission matrix of a phonon mode ω from one reservoir to the other. Remarkably, the expression is robust regardless of the complexity of the network and the number of particles that are attached to reservoirs and always satisfies the GC symmetry.

II. HARMONIC NETWORKS AND HEAT TRANSFER

We consider an arbitrary classical harmonic network with N positional degrees of freedom labeled $i = 1, 2, \dots, N$ of

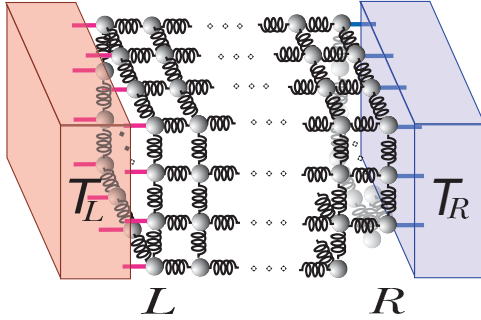


FIG. 1. (Color online) A schematic picture of the harmonic network connected to reservoirs. Positional degrees of freedom is labeled by $i = 1, \dots, N$. The points at $\ell = i \in L$ and $r = i \in R$ are attached to the left and right reservoirs.

which N_L are connected to a bath at temperature T_L and N_R are connected to a bath at temperature T_R (see Fig. 1). As an example, for a three-dimensional cubic crystal consisting of N_c^3 atoms with vector displacements, and with two opposite faces coupled to heat baths, we would have $N = 3N_c^3$ and $N_L = N_R = 3N_c^2$. We denote the positional degrees and their corresponding velocities by the column vectors $X = (x_1, x_2, \dots, x_N)^T$ and $V = (v_1, v_2, \dots, v_N)^T$, respectively. We consider the following general harmonic Hamiltonian for the system:

$$H = \frac{1}{2} V^T M V + \frac{1}{2} X^T K X, \quad (1)$$

where $M = \text{diag}\{m_1, m_2, \dots, m_N\}$ denotes the mass matrix and K the force matrix for the system. We model the heat baths by white-noise Langevin equations with each variable coupled to a bath having an independent Langevin dynamics. Let $L(R)$ refer to the set of $N_L(N_R)$ points connected to the left (right) bath. For discriminating these points from the bulk points, we use indices $\ell = i \in L$ and $r = i \in R$. We define the N -component noise vectors $\eta = \eta^{(L)} + \eta^{(R)}$ such that $\eta_\ell = \eta_\ell^{(L)}$ and $\eta_r = \eta_r^{(R)}$ are nonzero. Also we define the diagonal matrices $\boldsymbol{\gamma} = \boldsymbol{\gamma}^{(L)} + \boldsymbol{\gamma}^{(R)}$ such that $\gamma_{\ell\ell} = \gamma_{\ell\ell}^{(L)} \equiv \gamma_\ell$ and $\gamma_{rr} = \gamma_{rr}^{(R)} \equiv \gamma_r$ are nonzero. The equations of motion for the system are then given by

$$\begin{aligned} \dot{X} &= V, \\ M\dot{V} &= -KX - \boldsymbol{\gamma}V + \eta \\ &= -KX - \boldsymbol{\gamma}^{(L)}V + \eta^{(L)} - \boldsymbol{\gamma}^{(R)}V + \eta^{(R)}. \end{aligned} \quad (2)$$

The noise terms are assumed to be Gaussian white noise with zero mean and correlations given by $\langle \eta_\ell(t) \eta_{\ell'}(t') \rangle = 2\gamma_\ell T_L \delta_{\ell, \ell'} \delta(t - t')$, $\langle \eta_r(t) \eta_{r'}(t') \rangle = 2\gamma_r T_R \delta_{r, r'} \delta(t - t')$, and $\langle \eta_\ell(t) \eta_r(t') \rangle = 0$, where we have set the Boltzmann constant to the value one. The initial state at $t = 0$ is chosen from the steady-state distribution, and we measure the heat Q flowing

from the left reservoir into the system between the times $t = 0$ to $t = \tau$. We thus have

$$Q = \sum \int_0^\tau dt v_\ell (-\gamma_\ell v_\ell + \eta_\ell). \quad (3)$$

A solution of the linear equations Eq. (2) can be obtained by introducing the following discrete Fourier transforms and their inverses:

$$\begin{aligned} \{X(t), V(t), \eta(t)\} &= \sum_{n=-\infty}^{\infty} \{\tilde{X}(\omega_n), \tilde{V}(\omega_n), \tilde{\eta}(\omega_n)\} e^{-i\omega_n t}, \\ \{\tilde{X}(\omega_n), \tilde{V}(\omega_n), \tilde{\eta}(\omega_n)\} &= \frac{1}{\tau} \int_0^\tau \{X(t), V(t), \eta(t)\} e^{i\omega_n t}, \end{aligned}$$

where $\omega_n = 2\pi n/\tau$. Plugging these into Eq. (2), we get

$$\begin{aligned} \tilde{V}(\omega_n) &= -i\omega_n \mathbf{G}^+(\omega_n) [\tilde{\eta}^{(L)}(\omega_n) + \tilde{\eta}^{(R)}(\omega_n)] \\ &\quad + \frac{1}{\tau} \mathbf{G}^+(\omega_n) [K\Delta X + i\omega_n M\Delta V], \end{aligned} \quad (4)$$

$$\mathbf{G}^+(\omega_n) = [-M\omega_n^2 + K - \boldsymbol{\Sigma}^{(L)}(\omega_n) - \boldsymbol{\Sigma}^{(R)}(\omega_n)]^{-1}, \quad (5)$$

where $\boldsymbol{\Sigma}^{(L,R)}(\omega) = i\omega \boldsymbol{\gamma}^{(L,R)}$, $\Delta X = X(\tau) - X(0)$, and $\Delta V = V(\tau) - V(0)$. The matrix \mathbf{G}^+ is the Green's function connecting bulk variables with reservoir properties. The noise correlations in the Fourier space are given by

$$\begin{aligned} \langle \tilde{\eta}_\ell(\omega_n) \tilde{\eta}_{\ell'}(\omega_{n'}) \rangle &= 2\delta_{\ell, \ell'} \delta_{n, -n'} \gamma_\ell T_L / \tau, \\ \langle \tilde{\eta}_r(\omega_n) \tilde{\eta}_{r'}(\omega_{n'}) \rangle &= 2\delta_{r, r'} \delta_{n, -n'} \gamma_r T_R / \tau. \end{aligned} \quad (6)$$

Since the noise strength $\tilde{\eta}(\omega_n) \sim O(1/\tau^{1/2})$ and $\Delta X, \Delta V \sim O(1)$ we see that the second term in Eq. (4) is $\sim 1/\tau^{1/2}$ order smaller than the first and so can be dropped. It can in fact be shown that it contributes order $1/\tau$ corrections to the CGF [23]. We note that $\tilde{V}^*(\omega_n) = \tilde{V}(-\omega_n)$, $\tilde{\eta}^*(\omega_n) = \tilde{\eta}(-\omega_n)$. The heat transferred Q [Eq. (3)] can be expressed in terms of the Fourier modes with $n \geq 0$ as $Q = \sum_{n=0}^{\infty} \sum_{\ell} [-2\gamma_\ell \tilde{v}_\ell(\omega_n) \tilde{v}_\ell^*(\omega_n) + \tilde{\eta}_\ell(\omega_n) \tilde{v}_\ell^*(\omega_n) + \tilde{v}_\ell(\omega_n) \tilde{\eta}_\ell^*(\omega_n)]$. We define $\mathbf{G}^-(\omega) = \mathbf{G}^+(-\omega) = [\mathbf{G}^+(\omega)]^*$ and $\boldsymbol{\Gamma}^{(L,R)}(\omega) = \text{Im}[\boldsymbol{\Sigma}^{(L,R)}(\omega)] = \omega \boldsymbol{\gamma}^{(L,R)}$. On using the solution (4) without the second term, i.e., $\tilde{V}(\omega_n) = -i\omega_n \mathbf{G}^+(\omega_n) [\tilde{\eta}^{(L)}(\omega_n) + \tilde{\eta}^{(R)}(\omega_n)]$, we get the expression of Q as

$$\begin{aligned} Q &= \tau \sum_{n=0}^{\infty} (-2\omega_n) [\tilde{\eta}_{\ell'}(\omega_n) \mathbf{G}^+_{\ell\ell} + \tilde{\eta}_r(\omega_n) \mathbf{G}^+_{r\ell}] \boldsymbol{\Gamma}_{\ell\ell}^{(L)} \\ &\quad \times [\mathbf{G}_{\ell\ell'}^- \tilde{\eta}_{\ell'}^*(\omega_n) + \mathbf{G}_{\ell'r}^- \tilde{\eta}_r^*(\omega_n)] - i\omega_n \\ &\quad \times [\tilde{\eta}_{\ell'}(\omega_n) (\mathbf{G}_{\ell\ell'}^+ - \mathbf{G}_{\ell\ell}^-) + \tilde{\eta}_r(\omega_n) (\mathbf{G}_{r\ell}^+ - \mathbf{G}_{r\ell}^-)] \tilde{\eta}_\ell^*(\omega_n) \\ &= \tau \sum_{n=0}^{\infty} [\tilde{\eta}_L(\omega_n), \tilde{\eta}_R(\omega_n)] \mathcal{A} \begin{pmatrix} \tilde{\eta}_L^*(\omega_n) \\ \tilde{\eta}_R^*(\omega_n) \end{pmatrix}, \end{aligned} \quad (7)$$

where $\tilde{\eta}_L$ ($\tilde{\eta}_R$) denotes an N_L (N_R) component column vector of noise belonging to $\ell \in L$ ($r \in R$) sites, while the $N_L + N_R$ dimensional Hermitian matrix \mathcal{A} is given by

$$\mathcal{A} = \begin{pmatrix} 2\omega_n [\mathbf{G}^+ \boldsymbol{\Gamma}^{(R)} \mathbf{G}^-]_{LL} & i\omega_n [\mathbf{G}^-]_{LR} - 2\omega_n [\mathbf{G}^+ \boldsymbol{\Gamma}^{(L)} \mathbf{G}^-]_{LR} \\ -i\omega_n [\mathbf{G}^+]_{RL} - 2\omega_n [\mathbf{G}^+ \boldsymbol{\Gamma}^{(L)} \mathbf{G}^-]_{RL} & -2\omega_n [\mathbf{G}^+ \boldsymbol{\Gamma}^{(L)} \mathbf{G}^-]_{RR} \end{pmatrix}. \quad (8)$$

The subscripts L and R in the matrices, respectively, represent the space of ℓ and r sites. In Eqs. (7) and (8), the ω_n dependence of \mathbf{G} and $\mathbf{\Gamma}$ has been suppressed. In what follows, the ω_n dependence in variables is omitted unless it is necessary. In obtaining the (L, L) element of the matrix \mathcal{A} , we have used the following Green's function identity, which easily follows from the definition (5):

$$\begin{aligned} \mathbf{G}^+ - \mathbf{G}^- &= 2i\mathbf{G}^-(\mathbf{\Gamma}^{(L)} + \mathbf{\Gamma}^{(R)})\mathbf{G}^+ \\ &= 2i\mathbf{G}^+(\mathbf{\Gamma}^{(L)} + \mathbf{\Gamma}^{(R)})\mathbf{G}^-. \end{aligned} \quad (9)$$

III. CUMULANT GENERATING FUNCTION

We now proceed to the calculation of the CGF. The characteristic function $\mathcal{Z}(\lambda) = \langle e^{\lambda Q} \rangle$ is obtained by using the expression in Eq. (7) and averaging over the Gaussian noise variables, whose correlation matrix is given in Eq. (6). We get

$$\begin{aligned} \mathcal{Z}(\lambda) &= \mathcal{N} \prod_{n \geq 0} \int d[\tilde{\eta}_L, \tilde{\eta}_R, \tilde{\eta}_L^*, \tilde{\eta}_R^*] \exp \left\{ \tau (\tilde{\eta}_L, \tilde{\eta}_R) \right. \\ &\quad \left. \times \left[\lambda \mathcal{A} - \begin{pmatrix} \frac{1}{2T_L} [\mathbf{\Gamma}^{(L)}]^{-1} & 0 \\ 0 & \frac{1}{2T_R} [\mathbf{\Gamma}^{(R)}]^{-1} \end{pmatrix} \begin{pmatrix} \tilde{\eta}_L^* \\ \tilde{\eta}_R^* \end{pmatrix} \right] \right\}, \end{aligned} \quad (10)$$

where \mathcal{N} denotes the normalization factor of the noise distribution. By performing the Gaussian integral, one obtains the formal expression of the CGF:

$$\mu(\lambda) = \frac{1}{\tau} \log \mathcal{Z}(\lambda) \Big|_{\tau \rightarrow \infty} = -\frac{1}{\tau} \sum_{n \geq 0} \log \det \mathcal{B} \Big|_{\tau \rightarrow \infty}, \quad (11)$$

$$\mathcal{B} = \mathbf{1} - \lambda \begin{pmatrix} T_L & T_{LR} \\ T_{RL} & -T_R \end{pmatrix} \begin{pmatrix} T_L \mathbf{1} & \mathbf{0} \\ \mathbf{0} & T_R \mathbf{1} \end{pmatrix}, \quad (12)$$

where

$$\begin{aligned} T_L &= 4[\mathbf{G}^+\mathbf{\Gamma}^{(R)}\mathbf{G}^-\mathbf{\Gamma}^{(L)}]_{LL}, \\ T_R &= 4[\mathbf{G}^+\mathbf{\Gamma}^{(L)}\mathbf{G}^-\mathbf{\Gamma}^{(R)}]_{RR}, \\ T_{LR} &= -4[\mathbf{G}^+\mathbf{\Gamma}^{(R)}\mathbf{G}^-\mathbf{\Gamma}^{(L)}]_{LR} + 2i[\mathbf{G}^-\mathbf{\Gamma}^{(R)}]_{LR}, \\ T_{RL} &= -4[\mathbf{G}^+\mathbf{\Gamma}^{(L)}\mathbf{G}^-\mathbf{\Gamma}^{(L)}]_{RL} - 2i[\mathbf{G}^+\mathbf{\Gamma}^{(L)}]_{RL}. \end{aligned}$$

The matrices T_L and T_R are, respectively, $N_L \times N_L$ and $N_R \times N_R$ square matrices, and these can be regarded as transmission amplitude of energy with the mode ω_n from one reservoir to the other. For $N_L = N_R$, it is known that these matrices appear in the Landauer-like formula for average current [13]. As clarified later, even for unequal case $N_L \neq N_R$, both of these are transmission matrices and enter in the Landauer-like formula. Although the physical meaning of T_{LR} and T_{RL} are not clear, these are closely related to T_L and T_R . The relations can be revealed by using the relation (9) iteratively. Through tedious but straightforward calculations, one finds the following nontrivial relations:

$$T_{LR}T_R = T_L T_{LR}, \quad (13)$$

$$T_{RL}T_L = T_R T_{RL}, \quad (14)$$

$$T_{RL}T_{LR} = T_R(\mathbf{1} - T_R). \quad (15)$$

In order to get simple form of the CGF, we need to simplify the determinant of \mathcal{B} in Eq. (11). The relations (13)–(15) play a central role in simplifying the determinant of \mathcal{B} and in deriving the final expression of the CGF. We heuristically introduce the matrix \mathcal{C} :

$$\mathcal{C} = \begin{pmatrix} \mathbf{1} & C_{LR} \\ \mathbf{0} & C_{RR} \end{pmatrix}, \quad (16)$$

$$C_{LR} = \lambda T_R T_{LR} + \frac{T_R}{T_L} T_L T_{LR},$$

$$\begin{aligned} C_{RR} &= \mathbf{1} + \left(\frac{1}{\lambda T_L} - \lambda T_L - 1 \right) T_R + T_{RL} T_{LR} \\ &= \left(\mathbf{1} + \frac{T_R}{\lambda T_L} \right) (\mathbf{1} - \lambda T_L T_R). \end{aligned} \quad (17)$$

The advantage of introducing the matrix \mathcal{C} is that the product $\mathcal{B}\mathcal{C}$ has a simple form, and this is useful to simplify $\det \mathcal{B}$ given by $\det \mathcal{B}\mathcal{C} / \det \mathcal{C} = \det \mathcal{B}\mathcal{C} / \det C_{RR}$. With the relations (13)–(15), one finds the following form for the product:

$$\mathcal{B}\mathcal{C} = \begin{pmatrix} \mathbf{1} - \lambda T_L T_L & \mathbf{0} \\ -\lambda T_L T_{RL} & \left(\mathbf{1} + \frac{T_R}{\lambda T_L} \right) [\mathbf{1} - T_R T_L T_R \lambda (\lambda + \Delta\beta)] \end{pmatrix}, \quad (18)$$

and hence

$$\det \mathcal{B} = \det[\mathbf{1} - T_R T_L T_R \lambda (\lambda + \Delta\beta)] \frac{\det(\mathbf{1} - \lambda T_L T_L)}{\det(\mathbf{1} - \lambda T_L T_R)}. \quad (19)$$

Now by taking the singular value decomposition of the matrix $[(\mathbf{\Gamma}^{(L)})^{1/2} \mathbf{G}^+ (\mathbf{\Gamma}^{(R)})^{1/2}]_{LR}$ it can be shown that T_L and T_R have the same set of nonzero eigenvalues. Hence $\det(\mathbf{1} - \lambda T_L T_L) = \det(\mathbf{1} - \lambda T_L T_R)$, and on using this in Eq. (19) we get, in the large τ limit:

$$\mu(\lambda) = -\frac{1}{2\pi} \int_0^\infty d\omega \text{Tr} \log[\mathbf{1} - T(\omega) T_L T_R \lambda (\lambda + \Delta\beta)], \quad (20)$$

where one can use either T_L and T_R for the transmission matrix $T(\omega)$, both of which generate the same values of current cumulants. This formula for the CGF is the central result of this paper. One can easily check that the GC symmetry: $\mu(\lambda) = \mu(-\lambda - \Delta\beta)$ is satisfied. When the system is one dimensional and $N_L = N_R = 1$, the formula reproduces the classical limit of the quantum version of CGF [22]. Interestingly, the formula (20) is valid even for $N_L \neq N_R$. In this paper, for simplicity we demonstrated the derivation for baths with white Gaussian noise. However, the formula is also valid for generalized Langevin noise with memory kernel, with appropriate definition of the matrices $\mathbf{\Sigma}$ and $\mathbf{\Gamma}$.

IV. DISCUSSION

We have derived an exact formula for the CGF of a general harmonic network (20) and shown that it satisfies the GC symmetry. The formula is expressed in terms of the phonon transmission matrix. The CGF can be used to obtain the

average current $\langle Q \rangle_c / \tau$ and current noise $\langle Q^2 \rangle_c / \tau$ by taking the first and second derivatives with respect to λ :

$$\frac{\langle Q \rangle_c}{\tau} = \frac{(T_L - T_R)}{2\pi} \int_0^\infty d\omega \text{Tr}[\mathcal{T}(\omega)],$$

$$\frac{\langle Q^2 \rangle_c}{\tau} = \frac{1}{2\pi} \int_0^\infty d\omega \text{Tr}[\mathcal{T}^2(\omega)(T_R - T_L)^2 + 2\mathcal{T}(\omega)T_L T_R].$$

Higher-order cumulants are also systematically given.

The transmission matrix can be obtained either analytically or numerically. In case of higher-dimensional regular lattices, the recursive Green's function method can be used to efficiently generate the transmission matrix and thus evaluate the CGF. The disordered harmonic lattice shows different regimes of transport, such as ballistic, anomalous, and diffusive transports, and hence our result implies validity of the fluctuation theorem in all regimes of transport. In addition,

the formula (20) can be a powerful tool to explore generic features of current fluctuation in these different regimes. One of the most interesting possible application would be a test of the conjecture of the additivity principle [7].

An open problem is the quantum expression of the CGF. As in the one-dimensional case [22], a two-point observation protocol to get distribution of heat is necessary, and this seems to be a much more complex calculation than the one in this paper.

ACKNOWLEDGMENTS

We thank the Centre for Computational Science and Engineering, National University of Singapore, where this work was initiated. K.S. was supported by MEXT, Grant Number (21740288).

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