

Eigenstate thermalization to nonmonotonic distributions in strongly interacting chaotic lattice gases

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We find nonmonotonic equilibrium energy distributions, qualitatively different from the Fermi-Dirac and Bose-Einstein forms, in strongly interacting many-body chaotic systems. The effect emerges in systems with finite energy spectra, supporting both positive and negative temperatures, in the regime of quantum ergodicity. The results are supported by exact diagonalization calculations for chaotic Fermi-Hubbard and Bose-Hubbard models, when they have Wigner-Dyson statistics of energy spectra and demonstrate eigenstate thermalization. The proposed effects may be observed in experiments with cold atoms in optical lattices.

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I. INTRODUCTION

The properties of complex systems in thermodynamic equilibrium are determined by a few thermodynamic parameters, such as temperature, pressure, and density. Chaotic systems relax to equilibrium independently of their specific initial state. However, an isolated quantum system is described by the Schrödinger equation. Launching such a system in one of its eigenstates, it would remain in that state forever and the expectation value of any observable would be constant. This seems to violate the existence of a thermodynamic equilibrium state into which the system relaxes independently of its initial preparation.

The paradox is resolved by the eigenstate thermalization hypothesis (ETH) [1,2] (see also Refs. [3,4], the experimental work [5], the review [6], and the references therein). It states that the vast majority of a chaotic system's eigenstates behave as statistical ensembles and eigenstate expectation values already approximate the thermal equilibrium mean. More precisely, the expectation value of any local observable $\hat{O}$, evaluated for any eigenstate $|\alpha\rangle$ of a chaotic system, is approximately equal to its microcanonical mean over the pertinent energy shell,

$$\langle \alpha | \hat{O} | \alpha \rangle \approx \overline{\langle \alpha | \hat{O} | \alpha \rangle} \equiv \frac{\Delta_\alpha}{\Delta_{\text{MC}}} \sum_{\alpha' \in \text{MC}(E_\alpha)} \langle \alpha' | \hat{O} | \alpha' \rangle, \quad (1)$$

where E_α is the eigenstate energy, $\alpha \in \text{MC}(E)$ means that $|E_\alpha - E| < \Delta_{\text{MC}}/2$, Δ_{MC} is the microcanonical shell width, and Δ_α is the average distance between the adjacent $E_{\alpha'}$ in the vicinity of E_α .

Equation (1) provides an equilibrium state that is independent of the initial state details, but does not provide the equilibrium state properties. For a low-density gas of interacting particles in a flat potential, the equilibrium state agrees with the microcanonical ensemble for an ideal gas, as proven in Ref. [2] on the basis of the Berry conjecture [7] that each eigenfunction appears to be a superposition of plane waves with random phases and Gaussian random amplitudes, but fixed wavelength. In the thermodynamic limit, where the number of particles and the system's volume are increased while keeping a fixed particle density, the microcanonical ensemble provides the Fermi-Dirac (FD) or Bose-Einstein (BE) momentum distributions for the respective permutation symmetry, with the standard relation between the temperature and the total gas energy, which is equal to the eigenstate energy. Such distributions were also obtained for interacting Fermi [8,9] and Bose [10] systems close to quantum degeneracy, by appropriately shifting the microcanonical shell energies of the noninteracting system, effectively changing its temperature.

The eigenstates of the nonintegrable system are superpositions of the integrable-system eigenstates. The number of principal components (NPC) $\mathcal{N}_{\text{PC}}$ estimates (for each exact eigenstate) the number of contributing integrable-system eigenstates (see Appendix C). ETH means that the eigenstate-to-eigenstate fluctuations of expectation values within any chaotic microcanonical shell are suppressed. In certain situations [11,12], the fluctuation variance is inversely proportional to $\mathcal{N}_{\text{PC}}$. Thus, ETH typically implies large NPC, but can be practically attained when NPC is substantially smaller than the dimension $\mathcal{N}_{\text{HS}}$ of the Hilbert space (which can also be constrained due to possible conservation laws). NPC

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approaches a large fraction (limited by $1/3$ for time-reversible systems [13] or $1/2$ for time-irreversible ones [14]) of $\mathcal{N}_{\text{HS}}$ only in the regime of quantum ergodicity [15].

In this work, we demonstrate substantial qualitative deviations from the FD and BE distributions in certain strongly interacting, quantum-ergodic systems. These deviations go beyond any mapping between the microcanonical shells of the interacting and noninteracting systems (see, e.g., Ref. [10]), as the distributions become nonmonotonic.

Known deviations from the FD and BE distributions can be attributed to a lack of ergodicity. For example, quasi-integrable systems remember their initial state, as observed in experiments with quantum Newton cradles [16,17] and cold-atom breathers [18,19]. The relaxation outcomes for integrable systems are captured by generalized Gibbs ensembles [20] that account for additional integrals of motion. Incompletely chaotic systems [21,22] with a small number of degrees of freedom keep certain memory of their initial states. In many-body systems, eigenstate thermalization can also be prevented by many-body localization (MBL) [15,23], vanishing in the thermodynamic limit (see also, e.g., Refs. [24–27]). Even if ergodicity exists and eigenstate thermalization does take place, the distributions can deviate from the FD and BE ones due to moderate numbers of degrees of freedom in mesoscopic systems [28]. This effect, however, vanishes in large systems. Unlike all the above mechanisms, our results here are obtained in the quantum-ergodic regime and survive in large systems.

II. THE LATTICE MODELS

We find eigenstates of two lattice models by direct numerical diagonalization, allowed up to the Hilbert space dimension $\mathcal{N}_{\text{HS}} \lesssim 2 \times 10^4$. Throughout this manuscript, all energies are measured in units of the lattice hopping energy. In the first, two-dimensional (2D) Fermi-Hubbard (FH) model, N spin-polarized fermions have nearest-neighbor interactions with the strengths V (see Appendix A). This model includes hoppings with simultaneous change of l_x and l_y , which label sites of the $L_x \times L_y$ lattice. This, together with twisted periodic boundary conditions, allow us to remove degeneracies of the many-body noninteracting particle eigenstates. The total number of one-body (1B) states in this model is $L = L_x L_y$. Due to the spatial homogeneity of this model, we consider separately each sector with the given total momentum, which contains $\mathcal{N}_{\text{HS}} \approx (L-1)!/(N!(L-N)!)$ eigenstates. The results below are obtained for $N = 6$ particles in the 6×5 lattice ($L = 30$) and the total momentum x and y components 3 and 2, respectively. In this case, $\mathcal{N}_{\text{HS}} = 19811$.

The second model is a one-dimensional (1D) Bose-Hubbard (BH) chain with N spinless bosons in L sites, with on-site interactions of strength V and hard wall boundaries (see Appendix B). Parity symmetry is broken by adding a random disorder/bias potential of order ≤ 0.05 (see also Ref. [29]). The resulting Hilbert space dimension for the bosonic system is $\mathcal{N}_{\text{HS}} = (N+L-1)!/(N!(L-1)!)$. The system with $N = 10$ particles in $L = 8$ sites, considered here, has $\mathcal{N}_{\text{HS}} = 19448$.

Analyzing the chaotic system properties, we have to compare them to ones of the closest integrable system. For

this purpose, we use corresponding systems of noninteracting particles. Their symmetric or antisymmetric many-body eigenfunctions—the orbital Fock states $|n\rangle = |n_1, \dots, n_L\rangle$ —have the eigenenergies $E_n = \sum_k n_k \varepsilon_k$. Here, n_k are occupations of the 1B orbitals, labeled in increasing order of their eigenenergies ε_k . Subtracting the average expectation values of interactions from the interacting particle Hamiltonians (see Appendixes A and B) leads to a substantial overlap of the noninteracting and interacting spectra $\{E_n\}$ and $\{E_\alpha\}$.

III. EXACT DIAGONALIZATION RESULTS

For sufficiently strong interaction, both models become chaotic. For the FH model at $V = 1$, the ratio of two consecutive level spacings [30], averaged over the energy spectrum (see Appendix C), increases to $\langle r \rangle \approx 0.525$ (cf. $\langle r \rangle \approx 0.536$ [31] for the Wigner-Dyson ensemble of Gaussian orthogonal matrices, describing completely chaotic systems). The chaotic behavior is confirmed also by suppression of eigenstate-to-eigenstate fluctuations of the observable expectation values (see Appendix C). Their variances are reduced by two orders of magnitude. Another criterion of chaoticity, NPC, increased to 5×10^2 (see Appendix C). The chaoticity of the BH model is determined by the value of VN . For the BH model at $VN = 3.0$ ($V = 0.3$), we have $\langle r \rangle \approx 0.529$, fluctuation variances are reduced by two orders of magnitude, and NPC is increased to 8×10^2 . For these interaction strengths, the microcanonical distributions of the 1B orbital occupations [32] for interacting and noninteracting particles are very close (see Fig. 1). This is in line with Ref. [10], as subtracting the average expectation values of interactions from the interacting particle Hamiltonians is equivalent to the energy shift used there. We notice that both interacting and noninteracting distributions are different from the FD and BE distributions due to the small system size [28]. Due to macroscopic self-trapping, the BH model becomes integrable again at large V , where the site populations become effective integrals of motion. Thus, the chaoticity parameter reduces to $\langle r \rangle \approx 0.41$ at $V = 10$ (cf. $\langle r \rangle \approx 0.386$ for integrable systems).

In contrast, when the interaction is increased (but remains in the chaos region for the BH model), the microcanonical distributions for interacting particles deviate substantially from the noninteracting ones. This is shown in Fig. 1 for the FH model with $V = 10$, when $r \approx 0.53$ and NPC increases to the value of 6.2×10^3 , about one-third of $\mathcal{N}_{\text{HS}} = 19811$, and for the BH model with $V = 3$, $r \approx 0.5$, and NPC 4.5×10^3 (about one quarter of $\mathcal{N}_{\text{HS}} = 19448$). The selected energy shells represent the positive temperature range $E < (N/L) \sum \varepsilon_k$, where the distribution is monotonically decreasing with single-particle energy; the negative temperature range $E > (N/L) \sum \varepsilon_k$, where it is monotonically increasing; and the transition region between them, where it has a maximum for our small systems in the case of weak interactions [28]. Unlike the weak-interaction case, the interaction-energy shift implicit in our comparison (equivalent to Ref. [10]) does not capture the deviation, nor does any other energy shift, as the interacting and noninteracting distributions have different curvatures and are thus qualitatively different. As

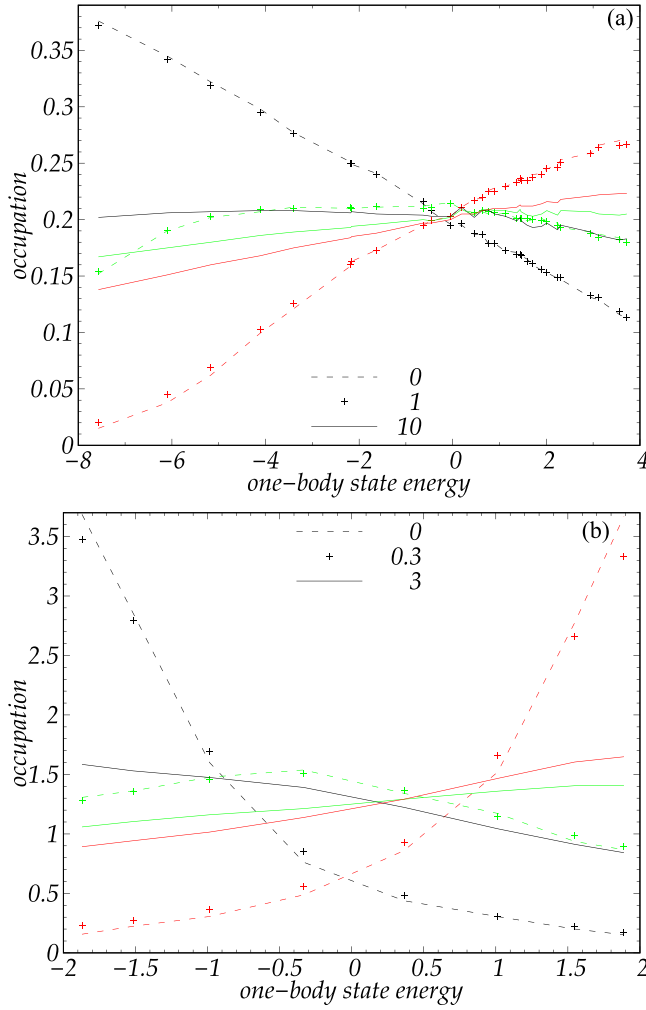


FIG. 1. 1B orbital occupations for (a) the FH model with the interaction strengths $V = 0$ (dashed lines), $V = 1$ (pluses), and $V = 10$ (solid lines), averaged over microcanonical shells with the mean energies -6 (black), 0 (green), and 6 (red) and (b) the 1D BH model with the interaction strengths $V = 0$ (dashed lines), $V = 0.3$ (pluses), and $V = 3$ (solid lines), averaged over microcanonical shells with the mean energies -1.2 (black), -0.17 (green), and 1.2 (red).

the eigenstate-to-eigenstate fluctuations are suppressed, the distributions for individual eigenstates deviate too.

IV. NONMONOTONIC DISTRIBUTIONS

The effect can be explained in the following way. Consider an observable $\hat{O}$ that commutes with the Hamiltonian of noninteracting particles, such that $\hat{O}|n\rangle = O_n|n\rangle$. The microcanonical mean (1) of its expectation value evaluated for eigenstates of interacting particles can be expressed as

$$\overline{\langle \alpha | \hat{O} | \alpha \rangle} = \sum_n \Delta_\alpha W(E, E_n) O_n \quad (2)$$

in terms of the local density of states (LDOS), or strength function [13]

$$W(E, E_n) = \frac{1}{\Delta_{MC}} \sum_{\alpha \in MC(E)} |\langle \alpha | n \rangle|^2 \quad (3)$$

[see Eq. (1)]. The LDOS is generally a flat function of energies. If its energy span Γ substantially exceeds Δ_{MC} , O_n in Eq. (2) is effectively averaged and can be approximated by its microcanonical mean

$$\overline{O}(E) = \frac{\Delta_n(E)}{\Delta_{MC}} \sum_{n \in MC(E)} O_n, \quad (4)$$

where $\Delta_n(E)$ is the average distance between neighboring E_n in the vicinity of E . Further, as Γ substantially exceeds Δ_n , approximating summation in Eq. (2) by integration, we get

$$\overline{\langle \alpha | \hat{O} | \alpha \rangle} \approx \int_{E_{\min}}^{E_{\max}} \frac{dE'}{\Delta_n(E')} \Delta_\alpha(E) W(E, E') \overline{O}(E'), \quad (5)$$

where $E_{\min}$ and $E_{\max}$ define the support of the noninteracting system's spectrum $E_{\{n\}}$.

Consider a particular case of the 1B orbital occupation operator $\hat{N}_k|n\rangle = n_k|n\rangle$, where k labels the 1B orbitals in increasing order of their eigenenergies ε_k (see Sec. II and Appendixes A and B). The microcanonical distribution of the orbital occupations for noninteracting particles $\overline{N}_k(E)$ is given by Eq. (4). The shape of $\overline{N}_k(E)$ depends on the mean shell energy E (see Fig. 1). If $W(E, E')$ vanishes when $|E - E'| > \Gamma$ and Γ is small with respect to the energy scale on which the microcanonical distribution $\overline{N}_k(E)$ varies, we can approximate the microcanonical distribution for interacting particles $\overline{N}_k^{\text{int}}(E) \equiv \overline{\langle \alpha | \hat{N}_k | \alpha \rangle}$ [see Eq. (5)] as $\overline{N}_k^{\text{int}}(E) \approx \overline{N}_k(E)$, thus justifying the equivalence between the occupation statistics of the interacting and noninteracting systems. However, if Γ exceeds this scale, the interacting system's occupation distribution $\overline{N}_k^{\text{int}}(E)$ can mix noninteracting distributions $\overline{N}_k(E)$ of different shapes and be different from any individual noninteracting microcanonical distribution $\overline{N}_k(E)$. In Fig. 1, mixing of increasing and decreasing $\overline{N}_k(E)$ leads to near uniform $\overline{N}_k^{\text{int}}(E)$.

The exact diagonalization method is applicable only to small numbers of particles and lattice sites when the microcanonical distribution of the orbital occupations $\overline{N}_k(E)$ is different from the FD and BE distributions [28]. However, for large numbers of noninteracting particles, the microcanonical and canonical thermodynamic means become equivalent (although the fluctuations in different ensembles can be nonequivalent even in the thermodynamic limit [33,34]). Then, the microcanonical occupations of the orbitals $\overline{N}_k(E)$ are precisely given by the FD or BE distributions,

$$\overline{N}_k(E) = (e^{(\varepsilon_k - \mu)/T} \pm 1)^{-1}, \quad (6)$$

where the chemical potential μ and temperature T are solutions to the system of equations $\sum_k \overline{N}_k(E) = N$ and $\sum_k \varepsilon_k \overline{N}_k(E) = E$. If ε_k is restricted from both below and above, T can be either positive or negative, corresponding to occupation distributions that decrease or increase, respectively, with the orbital energy. The summation over k in this system can be replaced by integration over the orbital energy. Then, μ and T will depend on the particle density $\tilde{N} = N/L$ and energy density $\tilde{E} = E/L$.

While finding the exact LDOS by direct diagonalization is not possible for large systems, in the case of strong interactions, it can be approximated by the Gaussian shape (see

Ref. [13]),

$$W(E, E_n) \approx C(E) \frac{\Delta_n(E_n)}{\Delta_n(E)} \exp(-(E - E_n)^2/\Gamma^2), \quad (7)$$

where $\Delta_n(E_n)$ is taken in the vicinity of E_n and the normalization factor $C(E)$ is determined by

$$1/C(E) = \int_{E_{\min}}^{E_{\max}} \exp(-(E - E')^2/\Gamma^2) dE'. \quad (8)$$

The Gaussian shape (7) approximates the LDOS with good accuracy even for systems of small size (see Appendix D). It should be stressed that the agreement can be provided by the factor $\Delta_n(E_n)$ even if the spectrum is substantially inhomogeneous. The resulting distributions, calculated with Eqs. (5)–(8), depend on scaled widths $\tilde{\Gamma} = \Gamma/L$. In addition to the 2D FH and 1D BH models, treated above using exact diagonalization, we consider also the 2D BH model with the same 1B Hamiltonian as the 2D FH one (see Appendix A). Figure 2 shows the obtained distributions for the Gaussian width Γ (increasing with the interaction strength V) covering both eigenstates corresponding to positive and negative temperatures, or, respectively, to the decreasing and increasing FD or BE distributions. The resulting distributions for the interacting system have clearly pronounced minima. This is provided by the positive second derivative $d^2\bar{N}_k(E)/d\varepsilon_k^2 > 0$ for the FD and BE distributions (6) when $(\varepsilon_k - \mu)/T > 0$. In contrast, for the few-mode systems of Fig. 1, the minimum does not appear due to a maximum of $\bar{N}_k(E)$ ($d^2\bar{N}_k(E)/d\varepsilon_k^2 < 0$) with $E \approx 0$, and the maximum vanishes in $\bar{N}_k^{\text{int}}(E)$ due to strong interactions.

Since $\mathcal{N}_{\text{PC}} \sim \Gamma/\Delta_n$ and $\mathcal{N}_{\text{HS}} \sim (E_{\max} - E_{\min})/\Delta_n$, the ratio of NPC to the Hilbert space dimension can be estimated as $\mathcal{N}_{\text{PC}}/\mathcal{N}_{\text{HS}} \sim \Gamma/(E_{\max} - E_{\min}) \approx \tilde{\Gamma}/(\tilde{N}\Delta\varepsilon)$, where the range of ε_k variation $\Delta\varepsilon$ is 12 for the 2D and 4 for the 1D models. Then, in Fig. 2, $\tilde{\Gamma} = 0.5$ corresponds to $\mathcal{N}_{\text{PC}}/\mathcal{N}_{\text{HS}} \sim 0.2$ for the 2D models and $\tilde{\Gamma} = 0.4$ corresponds to $\mathcal{N}_{\text{PC}}/\mathcal{N}_{\text{HS}} \sim 0.5$ for the 1D BH. These high participation fractions indicate quantum ergodicity [15].

V. DISCUSSION

It should be realized that Figs. 1 and 2 show the same effect, namely, the mixing of occupation distributions obtained from different microcanonical shells of the noninteracting system, due to a broadened LDOS. However, whereas in Fig. 2 the mean natural-mode occupations within microcanonical shells of the noninteracting system take the ubiquitous FD or BE forms (6), the corresponding distributions for few-mode mesoscopic system that can be numerically diagonalized as in Fig. 1 have nonuniversal and sometimes nonmonotonic structure in themselves [28]. The resulting strong-interaction occupation distribution is hence qualitatively different in the two cases. While numerical complexity precludes direct diagonalization for large systems, the nonmonotonic distributions in Fig. 2 are the inevitable result of the well-known FD or BE noninteracting shell distributions and the Gaussian line shape of the LDOS (7) that is confirmed in numerical calculations [13] and extends also to smaller systems (see Appendix D). Moreover, even this particular line shape is not necessary, as nonmonotonic

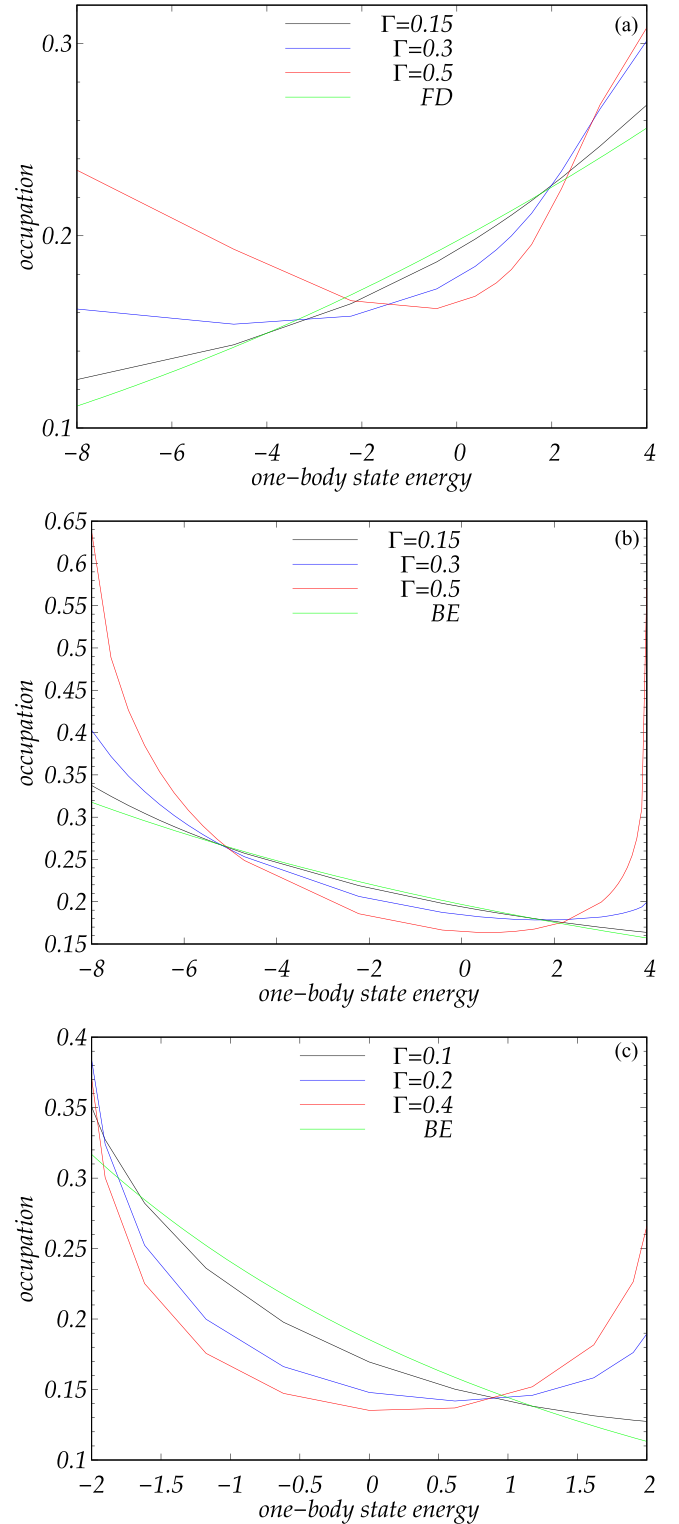


FIG. 2. 1B orbital occupations for different $\tilde{\Gamma}$. (a) The FH model with $\tilde{N} = 0.2$ and $\tilde{E} = 0.1$. (b) The 2D BH model with $\tilde{N} = 0.2$ and $\tilde{E} = -0.1$. (c) The 1D BH model with $\tilde{N} = 0.2$ and $\tilde{E} = -0.1$. The green lines show the FD or BE distributions corresponding to $\tilde{E}$.

distributions eventually appear for LDOS of any shape as long as it is sufficiently broadened by strong interactions.

In the MBL literature, the proportionality of NPC to Hilbert space dimension is used as an attribute of delocalization, distinguishing extended eigenstates from localized eigenstates. This property was reported for eigenstates in Heisenberg [35] and XXZ [36] spin chains, the Bose-Hubbard model [37], and the Jaynes-Cummings-Hubbard system [38]. Then, the ratio $\tilde{\Gamma}/\tilde{E} \sim \tilde{N}\Delta\epsilon\mathcal{N}_{\text{PC}}/(\mathcal{N}_{\text{HS}}\tilde{E})$ should remain unchanged for extended eigenstates in the thermodynamic limit $N \rightarrow \infty$, while $\tilde{N} = \text{const}$ and $\tilde{E} = \text{const}$. As a result, the distribution deviations from the FD and BE ones may survive in the thermodynamic limit.

For bosonic systems, there is a clear classical mean-field limit wherein the field operators are replaced by c numbers and their amplitudes and phases serve as conjugate action-angle canonical variables. The observed broadening of the LDOS may then be viewed as resulting from the interaction-induced deformation of the energy shells within the classical phase space. For the boson models discussed here, there is good quantum-classical correspondence in the sense that mean occupations agree well with semiclassical averages over the pertinent shells (see Refs. [28,39]) and the mean LDOS corresponds to the overlap of the classical shell of the noninteracting system with each of the interacting system's energy shells. While weak interactions only slightly shift the noninteracting shells, strong interactions deform them substantially: The noninteracting shell overlaps with many interacting shells, resulting in the broadening of the LDOS.

We reemphasize that the above deviations from the FD or BE distributions are quite different from those observed in Ref. [10]. The distributions presented in Fig. 2 therein are monotonic and agree perfectly with the BE distributions for the temperatures corresponding to the dressed energies. The dressed energy, given by Eq. (12) in Ref. [10], is shifted by the average expectation value of the interactions. As noted earlier, this prescription is implicit in all our calculations, as the average expectation values of the interactions are subtracted from the interacting system's eigenenergies (see Appendixes A and B). The deviations we observe are more profound than this simple energy shift. Our main point is that the interactions mix different microcanonical shells of the noninteracting system, so that the microcanonical occupation means over the interacting system's energy shell do not match any of the corresponding microcanonical means over noninteracting shells. This voids all energy-shift prescriptions, including that of Ref. [10]. The nonmonotonic distributions obtained here are a result of this mixing of shells with positive and negative temperatures and cannot be reduced to a change of temperature. Mixing of different shells was already considered in classical superstatistics [40] and thermodynamics of small systems [41], but with no relation to quantum eigenstates and nonmonotonic distributions.

VI. CONCLUSION

Orbital population distributions in eigenstates of strongly interacting many-body systems can be nonmonotonic and hence qualitatively deviate from the FD and BE distributions while the eigenstates are chaotic and thermalize. Unlike previously observed nonmonotonic occupation distributions

in weakly interacting mesoscopic systems [28], this strong-interaction effect appears due to the mixing of microcanonical shells with temperatures of opposite sign and survives in large systems. The distribution deviations may be observed experimentally with cold atoms in optical lattices.

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available upon publication because it is not technically feasible and/or the cost of preparing, depositing, and hosting the data would be prohibitive within the terms of this research project. The data are available from the authors upon reasonable request.

APPENDIX A: TWO-DIMENSIONAL LATTICE MODELS

The FH model on a two-dimensional (2D) lattice has the Hamiltonian

$$\hat{H}_F = - \sum_{l_x=1}^{L_x} \sum_{l_y=1}^{L_y} \sum_{\delta_x=-1}^1 \sum_{\delta_y=-1}^1 (1 - \delta_{\delta_x 0} \delta_{\delta_y 0}) \hat{a}_{l_x l_y}^\dagger \hat{a}_{l_x + \delta_x l_y + \delta_y} + \hat{V}_F - \bar{V}, \quad (\text{A1})$$

$$\hat{V}_F = V \sum_{l_x=1}^{L_x} \sum_{l_y=1}^{L_y} \left(\sum_{\delta_x=\pm 1} \hat{a}_{l_x l_y}^\dagger \hat{a}_{l_x + \delta_x l_y}^\dagger \hat{a}_{l_x l_y} \hat{a}_{l_x + \delta_x l_y} + \sum_{\delta_y=\pm 1} \hat{a}_{l_x l_y}^\dagger \hat{a}_{l_x l_y + \delta_y}^\dagger \hat{a}_{l_x l_y} \hat{a}_{l_x l_y + \delta_y} \right), \quad (\text{A2})$$

where V is the nearest-neighbor interaction strength, $\bar{V}$ is the average expectation values of the interactions $\hat{V}_F$ (see below), the hopping energy is used as the energy unit, $\hat{a}_{l_x l_y}$ are annihilation operators of spin-polarized fermions, and l_x, l_y specify location on the $L_x \times L_y$ lattice. Outside the square $1 \leq l_x \leq L_x, 1 \leq l_y \leq L_y$, the field operators are defined by the twisted periodic boundary conditions $\hat{a}_{l_x + L_x l_y} = e^{i\chi_x} \hat{a}_{l_x l_y}$ and $\hat{a}_{l_x l_y + L_y} = e^{i\chi_y} \hat{a}_{l_x l_y}$. The phase changes $\chi_x = (1 + \sqrt{5})/2$ (the golden ratio) and $\chi_y = e/2$ are used in the present calculations. The 1B orbitals are plane waves with the momentum components

$$p_x = \frac{2\pi m_x + \chi_x}{L_x} \quad (1 \leq m_x \leq L_x),$$

$$p_y = \frac{2\pi m_y + \chi_y}{L_y} \quad (1 \leq m_y \leq L_y), \quad (\text{A3})$$

where m_x and m_y are integers. The orbital energies are expressed as

$$\varepsilon_{2D}(p_x, p_y) = -2 \cos p_x - 2 \cos p_y - 4 \cos p_x \cos p_y. \quad (\text{A4})$$

The k th orbital momentum components $p_x(k)$ and $p_y(k)$ are chosen such that the orbitals are labeled in increasing order of their eigenenergies $\varepsilon_k = \varepsilon_{2D}(p_x(k), p_y(k))$. In the limit of the large $L_{x,y}$, the number of the orbitals with energies below ε ,

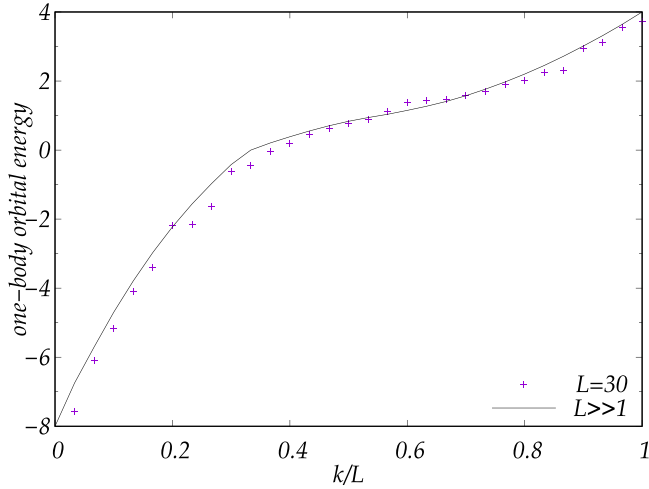


FIG. 3. One-body orbital energy as a function of the orbital label k for small and large FH models.

$k(\varepsilon)$, can be approximated by

$$\frac{k(\varepsilon)}{L} \approx \frac{1}{(2\pi)^2} \int_0^{2\pi} dp_x \int_0^{2\pi} dp_y \vartheta(\varepsilon - \varepsilon_{2D}(p_x, p_y)), \quad (\text{A5})$$

where summation over $m_{x,y}$ is approximated by integration over $p_{x,y}$, $L = L_x L_y$ is the total number of orbitals, and ϑ is the Heaviside step function. Inversion of $k(\varepsilon)$ allows us to express $\varepsilon_k = \varepsilon(k/L)$ in terms of lattice-size-independent function $\varepsilon(\tilde{k})$, which increases with $\tilde{k}$ from $\varepsilon(0) = -8$ to $\varepsilon(1) = 4$ (see Fig. 3).

The eigenstates of the Hamiltonian (A1) with $V = 0$ are thus the orbital Fock states $|n\rangle = |n_1, \dots, n_L\rangle$, where $0 \leq n_k \leq 1$ is the integer occupation of the k th orbital, and $\sum_{k=1}^L n_k = N$. Due to spatial homogeneity of the Hamiltonian (A1), we consider separately each segment with given total momentum components P_x and P_y , such that $\sum_{k=1}^L n_k p_{x,y}(k) = P_{x,y}$. The orbital Fock states for each segment constitute an $\mathcal{N}_{\text{HS}} \approx (L-1)!/(N!(L-N)!)$ -dimensional complete basis for the many-body Hilbert space with given P_x and P_y . Representing the full Hamiltonian in this basis and diagonalizing, we obtain the exact many-fermion eigenstates $|\alpha\rangle$.

The average expectation values of interactions $\bar{V} = \sum_{\alpha} \langle \alpha | \hat{V}_F | \alpha \rangle / \mathcal{N}_{\text{HS}}$ is subtracted in the Hamiltonian (A1) in order to provide a substantial overlap between the non-interacting and interacting spectra $\{E_n\}$ and $\{E_{\alpha}\}$. Due to completeness of the set $|\alpha\rangle$, we have

$$\bar{V} = \frac{1}{\mathcal{N}_{\text{HS}}} \sum_n \langle n | \hat{V}_F | n \rangle, \quad (\text{A6})$$

where diagonal matrix elements of the interaction (A2) can be expressed as

$$\begin{aligned} \langle n | \hat{V}_F | n \rangle = & \frac{4V}{L} \sum_{k < k'} n_k n_{k'} \left(\sin^2 \frac{p_x(k) - p_x(k')}{2} \right. \\ & \left. + \sin^2 \frac{p_y(k) - p_y(k')}{2} \right). \end{aligned} \quad (\text{A7})$$

As all orbitals are presented unbiasedly in the set $\{|n\rangle\}$, we can approximate the average over the Hilbert space in Eq. (A6) by the average over $p_x(k)$ and $p_y(k)$, i.e., replace squared sines in Eq. (A7) by $1/2$. As a result, we get

$$\bar{V} \approx 2N(N-1) \frac{V}{L}. \quad (\text{A8})$$

This approximate value will be valid as well for the average over each microcanonical interval, where the orbitals are presented unbiasedly. The stretching of the interacting spectrum $\{E_{\alpha}\}$ in comparison with the noninteracting one $\{E_n\}$ is related to the level repulsion, which is beyond the first-order effect in $\hat{V}_F$.

The expectation values of the orbital occupations $\langle \alpha | \hat{N}_k | \alpha \rangle$ for each of the $\mathcal{N}_{\text{HS}}$ eigenvalues are calculated with $\sum_{k=1}^L n_k m_x(k) = 3$, $\sum_{k=1}^L n_k m_y(k) = 2$, and $\mathcal{N}_{\text{HS}} = 19811$ for $N = 6$ particles in $L = 30$ sites of the 6×5 lattice.

We also consider a 2D BH model of the large system size. It has the Hamiltonian (A1), where $\hat{a}_{l_x l_y}$ are annihilation operators of spinless bosons and $\hat{V}_F$ is replaced by local interactions. The 1B Hamiltonian, orbitals, and ε_k for this model are the same as for the 2D FH one.

APPENDIX B: ONE-DIMENSIONAL BOSE-HUBBARD MODEL

The tight-binding bosonic Hamiltonian on a 1D lattice (in units of the hopping rate) reads

$$\hat{H}_B = - \sum_{l,m=1}^L \hat{b}_l^{\dagger} J_{lm} \hat{b}_m + \frac{1}{2} V \sum_{l=1}^L \hat{n}_l (\hat{n}_l - 1) - \bar{V}, \quad (\text{B1})$$

where $l = 1, \dots, L$ is the site index, $J_{lm} = J_{ml}^*$ is the hopping matrix coupling sites l and m , V is the on-site interaction strength, $\hat{n}_l = \hat{b}_l^{\dagger} \hat{b}_l$ is the number of bosons at site l , and $\hat{b}_l$ are bosonic particle annihilation operators. Throughout the manuscript, we have used the BH configuration $J_{l \neq m} = \delta_{l,m \pm 1}$ with hard wall boundaries, i.e., a linear chain of L sites. For this configuration, the dynamical behavior of the system, e.g., its degree of chaoticity, is set by the dimensionless interaction parameter $u = VN$. In order to remove the remaining parity symmetry and increase chaoticity, we have introduced a weak random “disorder” on-site potential $J_{l,l} = \text{rnd}[-0.05, 0.05]$.

The 1B orbitals are found by diagonalizing the hopping matrix, thereby obtaining the eigenvectors $\{f_{\alpha}\}_{\alpha=1,\dots,L}$ and the orbital energies ε_k . Defining the bosonic mode annihilation operators $\hat{c}_k = \sum_l f_k(l) \hat{b}_l$, where $f_k(l)$ denotes the l th component of the k th eigenvector, we obtain the orbital number operators:

$$\hat{N}_k = \hat{c}_k^{\dagger} \hat{c}_k = \sum_{l,m} f_k^*(l) f_k(m) \hat{b}_l^{\dagger} \hat{b}_m. \quad (\text{B2})$$

The BH Hamiltonian then transforms in the orbital basis into

$$\hat{H}_B = \sum_{k=1}^L \varepsilon_k \hat{c}_k^{\dagger} \hat{c}_k + \hat{V}_B - \bar{V}, \quad (\text{B3})$$

where

$$\hat{V}_B = \sum_{k,k',k'',k'''=1}^L u_{k,k',k'',k'''} \hat{c}_k^{\dagger} \hat{c}_{k'}^{\dagger} \hat{c}_{k''} \hat{c}_{k'''} \quad (\text{B4})$$

and

$$u_{k,k',k'',k'''} = \frac{V}{2} \sum_{i=1}^L f_k^*(i) f_{k'}^*(i) f_{k''}(i) f_{k'''}(i). \quad (\text{B5})$$

Note that in contrast to the FH model of the previous section, the system is not translationally invariant. Hence, there is no momentum conservation law that reduces the allowed four-wave-mixing transitions induced by the interactions between the orbitals.

The eigenstates of the Hamiltonian of Eq. (B3) with $V = 0$ are thus the orbital Fock states $|n\rangle = |n_1, \dots, n_L\rangle$, where n_k is the integer occupation of the k th orbital, and $\sum_{k=1}^L n_k = N$. The orbital Fock states constitute an $\mathcal{N}_{\text{HS}} = (N+L-1)!/(N!L!)$ -dimensional complete basis for the many-body Hilbert space (throughout the manuscript $\mathcal{N}_{\text{HS}} = 19448$ for $N = 10$ particles in $L = 8$ sites). Representing the full Hamiltonian in this basis and diagonalizing, we obtain the exact many-boson eigenstates $|\alpha\rangle$ and calculate the expectation values of the orbital occupations $\langle \alpha | \hat{N}_k | \alpha \rangle$ for each of the $\mathcal{N}_{\text{HS}}$ eigenvalues. In this model, $\bar{V} = \langle \alpha | \hat{V}_B | \alpha \rangle$ is the microcanonical mean of the interaction expectation value. For bosons, due to multiple orbital occupations, $\bar{V}$ is energy dependent. Then, it is numerically calculated for each microcanonical shell.

APPENDIX C: CHAOTIC PROPERTIES

The degree of chaoticity of a quantum system can be deduced from its level spacing statistics. One measure of the transition from the Poissonian statistics of integrable systems to the Wigner-Dyson statistics of completely chaotic systems is the ratio of consecutive level spacings

$$r_\alpha = \frac{\min(E_{\alpha+1} - E_\alpha, E_\alpha - E_{\alpha-1})}{\max(E_{\alpha+1} - E_\alpha, E_\alpha - E_{\alpha-1})} \quad (\text{C1})$$

averaged over the entire spectrum or over a pertinent energy shell. This criterion has been introduced in Ref. [30], and is very widely used as a clear evidence of integrability-chaos transition. The value $\langle r \rangle = 2 \ln 2 - 1 \approx 0.38629$ is indicative of Poissonian statistics, whereas $\langle r \rangle = 4 - 2\sqrt{3} \approx 0.53590$ is obtained for Wigner-Dyson Gaussian orthogonal ensemble (GOE) statistics [31]. In Fig. 4, we present this measure as a function of the interaction strength for our model systems. The 1D BH system is integrable at weak interaction due to its near-separability and at strong interaction due to macroscopic self-trapping, where site occupations become integrals of motion. In contrast, the 2D FH system does not return to integrability at high interaction strength. Figure 4 presents also another characteristic of chaos—the NPC, or the participation ratio, $\mathcal{N}_{\text{PC}} = \eta^{-1}$, where the inverse participation ratio is defined by

$$\eta = \sum_n | \langle n | \alpha \rangle |^4. \quad (\text{C2})$$

In Fig. 4(a), $\mathcal{N}_{\text{PC}} \approx 6.2 \times 10^3$ for $V = 10$ and $\mathcal{N}_{\text{PC}} \approx 6.5 \times 10^3$ for $V = 20$, tending to the GOE limit $\mathcal{N}_{\text{HS}}/3 \approx 6.6 \times 10^3$ at $V \rightarrow \infty$.

Note that a high NPC is a necessary but not sufficient condition for chaos, as the number of eigenstates of a

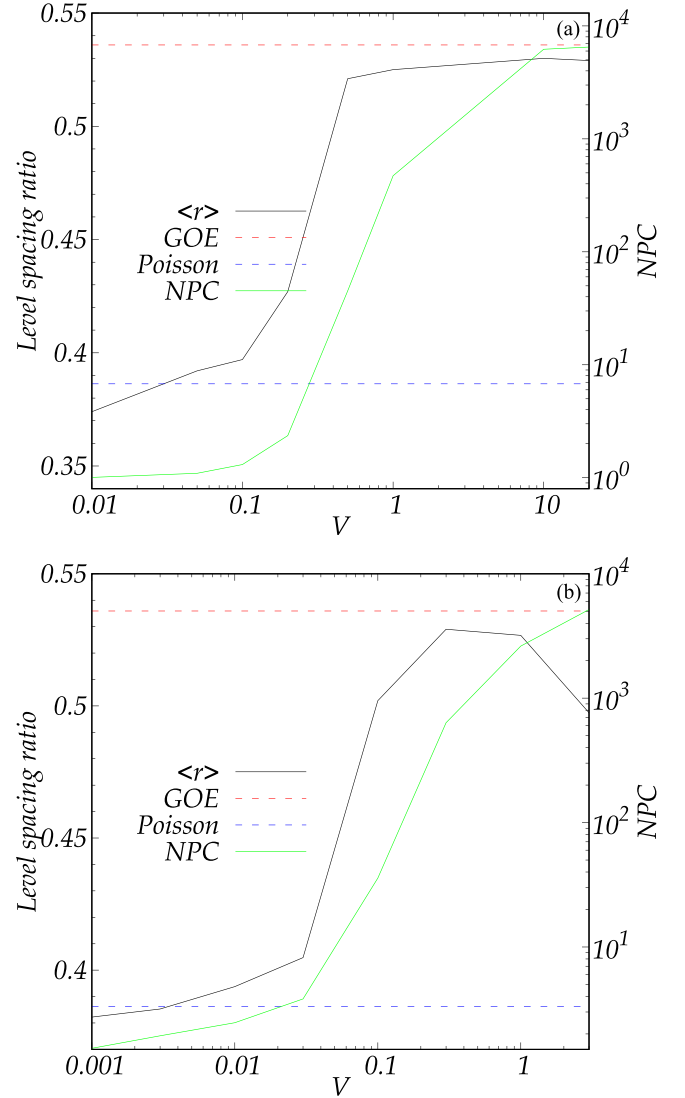


FIG. 4. (a) Level spacing ratio (black line) vs interaction strength for the FH model. Dashed lines show $\langle r \rangle$ for the Poisson and GOE statistics. The green line shows NPC. (b) The same for the 1D BH model.

noninteracting system participating in an eigenstate of the interacting system can be large even if the latter is integrable.

Chaos can also be characterized by the eigenstate-to-eigenstate fluctuations of the observable expectation values. The fluctuation variances for an observable $\hat{O}$ are expressed as

$$\text{Var}_\alpha(\hat{O}) = \overline{\langle \alpha | \hat{O} | \alpha \rangle^2} - \overline{\langle \alpha | \hat{O} | \alpha \rangle}^2. \quad (\text{C3})$$

The variances are presented in Fig. 5. Due to the large number of the orbitals in the FH model, we consider cumulative observables: the total occupations of orbitals with $m_x < L_x/2$ and any m_y in Eq. (A3) [low x in Fig. 5(a)], with $m_y < L_y/2$ and any m_x (low y), with $m_x < L_x/2$ and $m_y < L_y/2$ (low xy), with even m_x and any m_y (even x), with even m_y and any m_x (even y), and with even m_x and m_y (even xy). We also consider

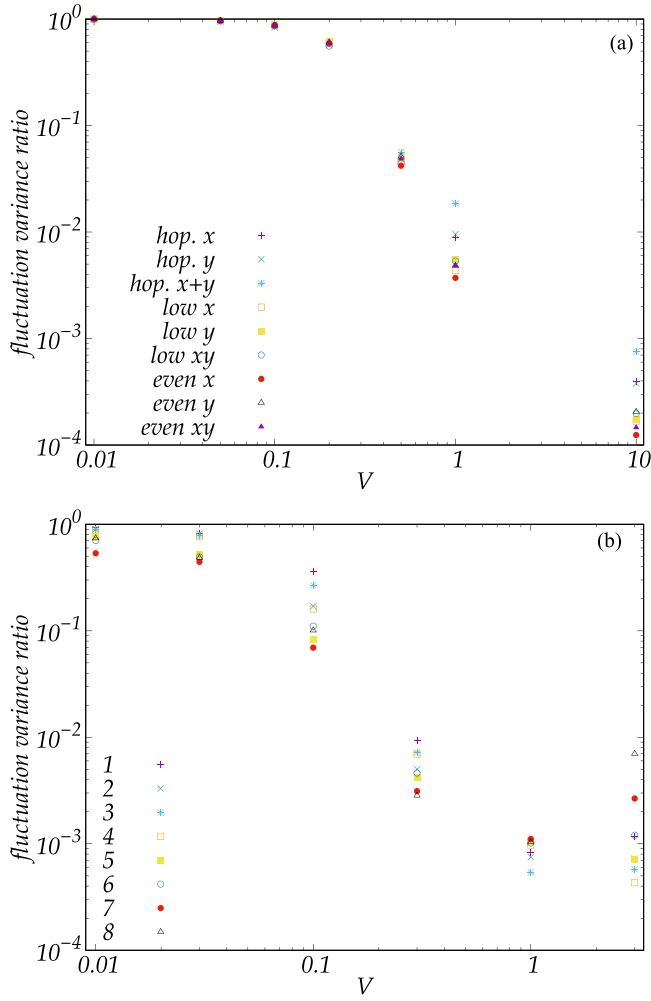


FIG. 5. Ratio of eigenstate-to-eigenstate fluctuation variances for the nonintegrable to ones for the integrable systems eigenstates vs interaction strength for (a) the FH model averaged over the micro-canonical shell with the mean energy 0 and (b) the 1D BH model with the mean shell energy -5.14 .

the hopping energies in the x and y directions

$$\begin{aligned}
 & - \sum_{l_x=1}^{L_x} \sum_{l_y=1}^{L_y} \sum_{\delta_x=\pm 1} \hat{a}_{l_x l_y}^\dagger \hat{a}_{l_x+\delta_x l_y} \\
 & - \sum_{l_x=1}^{L_x} \sum_{l_y=1}^{L_y} \sum_{\delta_y=\pm 1} \hat{a}_{l_x l_y}^\dagger \hat{a}_{l_x l_y+\delta_y},
 \end{aligned}$$

as well as the sum of these energies. For the 1D BH model, due to the small number of orbitals, we consider the individual orbital occupations.

APPENDIX D: LOCAL DENSITY OF STATES

Figure 6 demonstrates the LDOS (see Ref. [6]) averaged over the orbitals

$$\bar{W}(E, \bar{E}_n) = \frac{\Delta_n(E_n)}{\Delta_{MC}} \sum_{n \in MC(\bar{E}_n)} W(E, E_n)$$

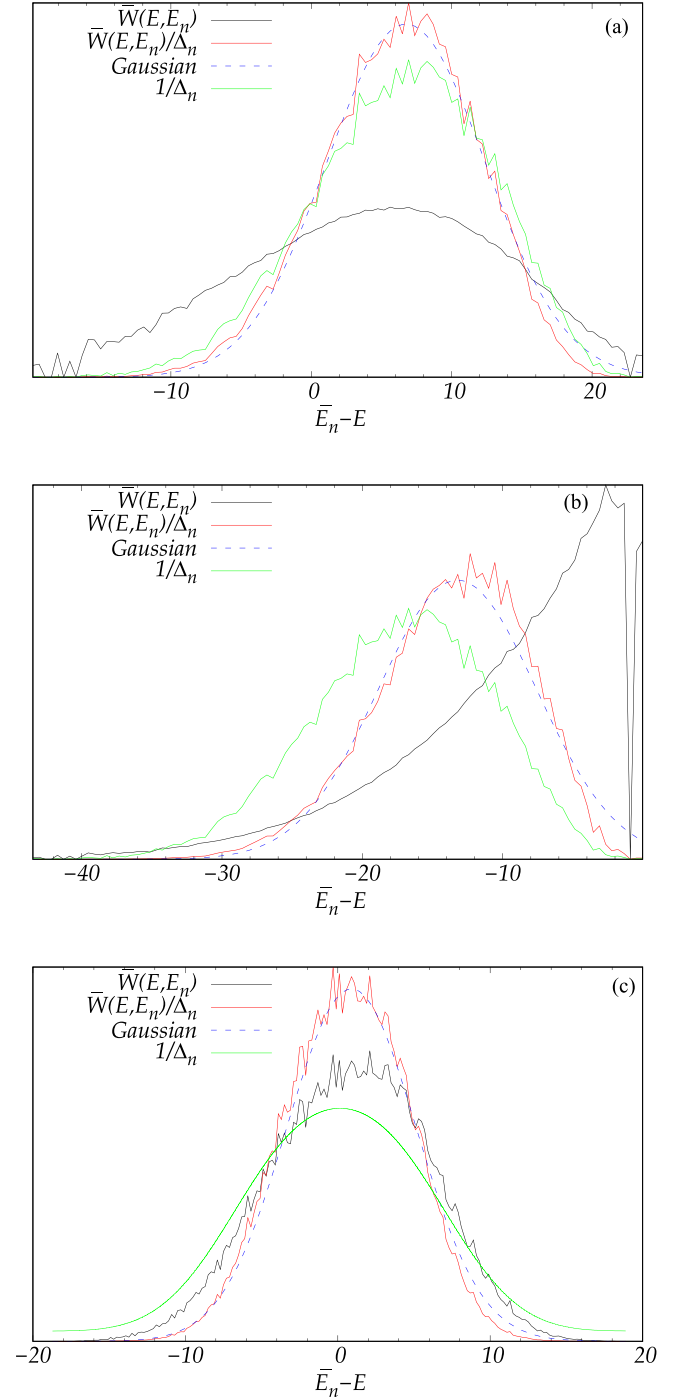


FIG. 6. Local density of states, averaged over the orbitals, for (a) the FH model with $V=10$ at $E=-5.2$, (b) the FH model with $V=10$ at $E=38.4$, and (c) the 1D BH model with $V=3$ at $E=-5.14$.

and the averaged LDOS divided by $\Delta_n(E_n)$ in a comparison with the Gaussian profiles.

In the center of the spectrum, both $\bar{W}(E, \bar{E}_n)$ and $\bar{W}(E, \bar{E}_n)/\Delta_n(E_n)$ can be approximated by Gaussian profiles [see Figs. 6(a) and 6(c)]. However, near the spectrum boundaries, where the spectrum is substantially inhomogeneous, only $\bar{W}(E, \bar{E}_n)/\Delta_n(E_n)$ has a Gaussian shape, but $\bar{W}(E, \bar{E}_n)$ does not [see Fig. 6(b)].

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