

# Bound on Eigenstate Thermalization from Transport

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We show that presence of transport imposes constraints on matrix elements entering the Eigenstate Thermalization Hypothesis (ETH) ansatz and require them to be correlated. It is generally assumed that the ETH ansatz reduces to Random Matrix Theory (RMT) below the Thouless energy scale. We show this conventional picture is not self-consistent. We prove that the energy scale at which ETH ansatz reduces to RMT has to be parametrically smaller than the inverse timescale of the slowest thermalization mode present in the system. In particular it has to be parametrically smaller than the Thouless energy. Our results indicate there is a new scale relevant for thermalization dynamics.

Thermalization of isolated quantum systems has attracted significant attention recently. For the quantum ergodic systems without local integrals of motion it is currently accepted that thermalization can be explained with the help of the Eigenstate Thermalization Hypothesis (ETH) [1–8]. At the technical level ETH can be understood as an ansatz for the matrix elements of observables in the energy eigenbasis [5],

$$A_{ij} = A^{\text{eth}}(E)\delta_{ij} + \Omega^{-1/2}(E)f(E,\omega)r_{ij} , \quad (1)$$

$$E = (E_i + E_j)/2 , \quad \omega = E_i - E_j . \quad (2)$$

Here  $A$  is an observable satisfying ETH,  $\Omega(E)dE$  is the density of states,  $A^{\text{eth}}$  and  $f$  are smooth functions of their arguments, and  $r_{ij}$  are pseudo-random fluctuations with the magnitude one. The diagonal part of the ETH ansatz explains thermalization, at least in the sense that the expectation value of  $A$  in some state of mean energy  $E$ , averaged over time, is equal to the thermal expectation value with effective temperature  $\beta^{-1}(E) = d \ln \Omega / dE$ . The dynamics of thermalization is encoded in the off-diagonal matrix elements  $r_{ij}$ , as well as in the initial state  $\Psi$ , and is not universal. In this paper we show that the locality of interactions imposes constraints on the  $r_{ij}$ , which depend on the type of transport present in the system.

Numerical studies confirm that the  $r_{ij}$  behave “randomly” and oscillate around zero mean seemingly without any obvious pattern. Certainly the  $r_{ij}$  can not be random in the literal sense as the form of  $A_{ij}$  is fixed once the Hamiltonian and  $A$  are specified. Moreover,  $A$  often has to satisfy various algebraic relations. For example, in a spin lattice model one can choose  $A$  to be a Pauli matrix acting on a particular site. In this case  $A^2 = \mathbb{I}$ , which requires  $r_{ij}$  to be correlated. Similarly, the  $r_{ij}$  can be constrained by the expected behavior of the four-point correlation function [9], etc.

While the whole matrix  $r_{ij}$  can not be random, there is an expectation that fluctuations  $r_{ij}$  can be treated as such if the indexes  $i, j$  are restricted to belong to a suffi-

ciently narrow energy interval. Assuming the interval is centered around some  $E$ , we define  $\Delta E_{\text{RMT}}$  as the largest possible interval size such that  $r_{ij}$  for  $i, j$  constrained by

$$|E_k - E| \leq \Delta E_{\text{RMT}} , \quad k = i, j , \quad (3)$$

can be treated for physical purposes as being random and independent (without necessary being normally distributed). The expectation that  $r_{ij}$  reduces to a Gaussian Random Matrix inside a sufficiently narrow interval is consistent with numerical studies which confirm that the  $r_{ij}$  are normally distributed [10–12] and that the form-factor  $f$  becomes constant for  $\omega$  smaller than the Thouless energy  $\Delta E_{\text{Th}}$  [13–16]. Furthermore, for real symmetric  $A_{ij}$  the variances of the diagonal and off-diagonal elements have been numerically shown to satisfy  $\langle r_{ii}^2 \rangle = 2\langle r_{ij}^2 \rangle$  [17, 18], which is consistent with and necessary for the  $r_{ij}$  being a GOE. Random behavior of  $r_{ij}$  also naturally emerges in a recent attempt to justify ETH analytically [19]. From the physical point of view the “structureless” form of  $A_{ij}$  inside a small energy interval is expected on the grounds of the hypothetical universal behavior of observables at late times [20–22]. The conventional picture of thermalization of ergodic systems with an approximate translational symmetry suggests that the system is fully thermalized after the Thouless time  $\Delta E_{\text{Th}}^{-1}$ , necessary for the slowest transport mode to propagate across the system. Thus, for systems with diffusive transport and characteristic size  $L$  one expects that after time  $t \sim L^2$  the system is fully ergodic in the sense that local physical observables do not depend on the initial state. This qualitative picture suggests that  $r_{ij}$  should become structureless for  $\Delta E_{\text{RMT}} \sim \Delta E_{\text{Th}} \sim 1/L^2$  [14]. We show below this is not the case, and  $\Delta E_{\text{RMT}}$  has to be parametrically smaller than the Thouless energy  $\Delta E_{\text{Th}}$ . Our findings raise the question of identifying the correct scaling of  $\Delta E_{\text{RMT}}$  with the system size and understanding the significance of the associated timescale  $\Delta E_{\text{RMT}}^{-1}$  from the point of view of thermalization dynamics.

Systems with local interactions have a finite maximal velocity of physical signals [23, 24]. As a result a quasi-classical configuration with an extensive amount of energy distributed locally would require at least time  $t \gtrsim L$  to thermalize. To avoid possible subtleties due to possible large energy variance of the initial state, in which case the system may equilibrate, but will not thermalize, we construct the initial state explicitly. For concreteness we consider a one-dimensional spin lattice model of length  $L$  with short-range interactions. We split the system into two non-interacting subsystems of approximately equal lengths  $L/2$  by removing the corresponding interaction terms from the original Hamiltonian  $H$ . The desired initial state can be chosen as a tensor product  $|\Psi\rangle = |E_-\rangle \otimes |E_+\rangle$  of two energy eigenstates of the corresponding subsystems. By choosing different  $E_-$  and  $E_+$  with an extensive difference  $|E_+ - E_-| \sim L$ , one creates a configuration of two adjacent subsystems with different effective temperatures. We will show now that it will take an extensive time for this state to thermalize. Indeed,  $|\Psi\rangle$  is an eigenstate of the Hamiltonian  $H_0$ , which is the original Hamiltonian  $H$  with the interactions between the two subsystems removed. Hence, from the point of view of the original Hamiltonian the energy variance of  $|\Psi\rangle$  is bounded by the norm of  $H_{\text{int}} = H - H_0$  which is sub-extensive. In terms of the decomposition

$$|\Psi\rangle = \sum_i C_i |E_i\rangle, \quad (4)$$

where  $|E_i\rangle$  are the eigenvalues of  $H$ , this means that most  $|E_i\rangle$  contributing to (4) will correspond to the same energy density and therefore this state will thermalize rather than merely equilibrate [6]. To describe the time evolution of  $|\Psi\rangle$  it is convenient to first switch to the Heisenberg picture and then employ the interaction picture splitting  $H$  into  $H_0 + H_{\text{int}}$ . Then the thermalization of  $|\Psi\rangle$  is due to the growth of the local operator  $H_{\text{int}}$  under the time-evolution induced by  $H_0$ . For a local operator  $A$  located a distance  $z$  away from the location of  $H_{\text{int}}$  in the center of the chain the Lieb-Robinson bound [23] guarantees that  $\langle \Psi | A(t) | \Psi \rangle$  will remain constant to within an exponential precision at least up to times  $t \sim z$ . Unless the thermal expectation value  $\langle A \rangle_\beta$  of  $A$  is identically the same for all temperatures, the deviation

$$\delta A(t, \Psi) = \langle \Psi | A(t) | \Psi \rangle - A^{\text{eth}}(E_\Psi), \quad E_\Psi = \langle \Psi | H | \Psi \rangle, \quad (5)$$

will have a non-zero  $L$ -independent value at  $t = 0$  and will remain approximately the same for times  $t \gtrsim z \sim L$ , after which it will go to zero. In other words we have shown that the expectation value of a general local operator  $A$  in the state  $\Psi$  will take an extensive time  $\tau \gtrsim L$  to relax to its thermal value. (For local operators  $A$  located near the middle point  $z \ll L$  it is easy to construct a somewhat different initial  $|\Psi\rangle$  reaching the same conclusion.)

The key observation of this paper is that the ETH ansatz (1) with random mutually-independent  $r_{ij}$  is constrained by presence of states with long thermalization times. The strongest constraint is provided by the slowest mode probed by  $A$ . If the system exhibits diffusive transport, provided  $A$  is coupled to the diffusive quantity, the time that the deviation (5) will remain of order one is even longer,  $t \sim L^2$ . In one dimensions the step-like profile discussed above can be decomposed into Fourier series with the  $n$ -th harmonics decaying as  $e^{-n^2 D t / L^2}$ , where  $D$  is the diffusion coefficient. At late times only the slowest mode survives with (5) behaving as  $\sim e^{-t/\tau}$ ,  $\tau = L^2/D$ . This quasi-classical behavior for the state  $|\Psi\rangle$  described above was recently confirmed numerically in [25]. In what follows we will focus on the constraints provided by the diffusive modes. A generalization for different types of transport is straightforward.

To connect thermalization time to matrix elements of  $A$  we introduce a  $T$ -dependent average quantity, which is conceptually similar to the ‘‘average distance’’ used in [26] to characterize thermalization time,

$$\langle \delta A \rangle_T \equiv \int_{-\infty}^{\infty} \delta A(t, \Psi) \frac{\sin(\pi t/T)}{\pi t} dt. \quad (6)$$

Here  $T$  is a free parameter. When the thermalization time  $\tau$  of  $\Psi$ , which is the characteristic time necessary for  $\delta A(t)$  to become zero, is smaller than  $T$ , (6) reduced to the conventional average over time  $T$ ,

$$\langle \delta A \rangle_T \approx \frac{1}{T} \int_{-T/2}^{T/2} \delta A(t, \Psi) dt. \quad (7)$$

After performing the integral in (6) using (1) we find

$$\langle \delta A \rangle_T = \langle \Psi | A_T | \Psi \rangle + \sum_i |C_i|^2 (A^{\text{eth}}(E_i) - A^{\text{eth}}(E_\Psi)), \quad (8)$$

where the operator  $A_T$  written in the energy eigenbasis has the form

$$(A_T)_{ij} = \begin{cases} \Omega^{-1/2}(E) f(E, \omega) r_{ij}, & |E_i - E_j| \leq \pi/T \\ 0, & |E_i - E_j| > \pi/T \end{cases} \quad (9)$$

In other words the matrix  $(A_T)_{ij}$  has a band structure, it coincides with  $A_{ij}$  (after subtracting the non-random diagonal part) inside a diagonal band of size  $\pi/T$ , and is zero outside. This is schematically shown in Fig. 1.

For systems admitting a thermodynamic limit the function  $A^{\text{eth}}(E)$  is a smooth function of the energy density  $E/V$ . Second term in (8) is small, it scales with the volume as  $\mathcal{O}(\Delta E_\Psi/V)$ , where  $\Delta E_\Psi$  is the energy variance of  $|\Psi\rangle$ . In our case this is  $\mathcal{O}(1/L)$ , which is also the discrepancy between different definitions of thermal expectation value of  $A$  in 1D. First term  $\langle \Psi | A_T | \Psi \rangle$  can be bounded by the largest eigenvalue of  $(A_T)_{ij}$ . Let us define the function  $x(E, \Delta E, T)$  to be the maximal (by

absolute value) eigenvalue of the sub-matrix  $(A_T)_{ij}$  with indices  $i, j$  satisfying

$$|E_k - E| \leq \Delta E, \quad k = i, j. \quad (10)$$

When  $\Delta E$  is smaller than  $\pi/(4T)$ , i.e. the sub-matrix is fully inside the band, the inverse of  $x(E, \Delta E, T)$  reduces to the canonical universality function  $\Delta E(x)$  introduced in [17]. Since the initial state  $|\Psi\rangle$  has sub-extensive energy variance, for physical purposes we assume  $|\Psi\rangle$  can be restricted to belong to some large but sub-extensive energy interval. Then  $\langle \Psi | A_T | \Psi \rangle$  in (8) can be bounded by  $x(E_\Psi, \Delta E, T)$  with a sufficiently large but sub-extensive  $\Delta E \ll E_\Psi$ . We show in the appendix that in full generality maximal eigenvalue  $x(E_\Psi, \Delta E, T)$  is bounded by

$$x(E_\Psi, \Delta E, T) \leq 2x(E', \pi/(2T), T) + x(E'', \pi/(4T), T), \quad (11)$$

where  $E'$  and  $E''$  are some energies inside the interval  $[E_\Psi - \Delta E, E_\Psi + \Delta E]$ . On physical grounds we expect  $x(E, \Delta E)$  to depend on energy density  $E/V$  specifying effective temperature, and theretofore the precise values of  $E', E''$  are unimportant.

Let us assume now that  $T$  is sufficiently large such that  $\pi/(2T) \leq \Delta E_{\text{RMT}}$ . Then the sub-matrices  $(A_T)_{ij}$  associated with  $x(E', \pi/(2T), T)$  and  $x(E'', \pi/(4T), T)$  are small enough to satisfy  $\Delta E_{\text{RMT}} \geq \Delta E$ . Then the corresponding sub-matrices are band random matrices with independent (but not necessarily normally distributed)  $\delta A_{ij}$  and their respective largest eigenvalues are controlled by the variance function  $\overline{\delta A_{ij}^2}(\omega)$  [27]. In particular largest eigenvalue satisfies the inequality [17]

$$x^2(E, \Delta E, T) \leq 8 \int_0^{\pi/(2T)} f^2(E, \omega) d\omega. \quad (12)$$

Here we have assumed that  $\beta \Delta E \ll 1$  so that the density of states  $\Omega(E)$  within the interval (10) can be taken to be constant. The inequality (12) is a uniform bound which does not depend on  $\Delta E$  provided  $\Delta E \geq \pi/(4T)$ , i.e. the sub-matrix is wider than the band. With help of (1) the integral (12) can be related to the connected autocorrelation function of  $A$  associated with the effective inverse temperature  $\beta^{-1} = d \ln \Omega / dE$  [13–15],

$$\langle A(t)A(0) \rangle_\beta \equiv \langle E | A(t)A(0) | E \rangle - \langle E | A^2(0) | E \rangle. \quad (13)$$

Combining everything together and ignoring for now the  $\mathcal{O}(1/L)$  contribution from the second term of (8), we find the inequality

$$\left| \int_{-\infty}^{\infty} \delta A(t, \Psi) \frac{\sin(\pi t/T)}{\pi t} dt \right|^2 \leq 36 \int_{-\infty}^{\infty} \langle A(t)A(0) \rangle_\beta \frac{\sin(\pi t/(2T))}{\pi t} dt, \quad (14)$$

$$\beta^{-1} = d \ln \Omega / dE \Big|_{E_\Psi}, \quad (15)$$

which should be satisfied for  $T \geq \pi/(2\Delta E_{\text{RMT}})$ .

The inequality (14) is our main technical result, which implies strong limitations on  $\Delta E_{\text{RMT}}$ . We first notice that the right-hand-side of (14) becomes very small for large  $T$  even after taking thermodynamic limit. Assuming the effective temperature  $\beta$  remains fixed as we scale the size of the system to infinity, the autocorrelation function of a local diffusive operator  $A$  normally behaves as  $\langle A(t)A(0) \rangle_\beta \sim (t_D/|t|)^\alpha$  for large  $t \gg t_D$ , where constants  $\alpha > 0$  and  $t_D$  are  $L$ -independent. Thus, for 1D diffusive systems  $\alpha = 1/2$  and  $t_D$  is related to the diffusion constant at temperature  $\beta^{-1}$ . The polynomial decay of  $\langle A(t)A(0) \rangle_\beta$  is believed to persist until the Thouless time  $\tau \sim L^2/D$ , after which the two-point function becomes zero [14, 15]. Hence for  $T \gg t_D$ , up to an unimportant overall numerical coefficient, the right-hand-side of (14) can be approximated as

$$\int_{-\infty}^{\infty} \langle A(t)A(0) \rangle_\beta \frac{\sin(\pi t/(2T))}{\pi t} dt \sim \begin{cases} \sqrt{t_D/T}, & \tau \gtrsim T \gg t_D \\ \sqrt{t_D \tau}/T, & T \gtrsim \tau \end{cases} \quad (16)$$

For large  $T \gg t_D$  (16) is very small for any value of  $\tau$ . The behavior of the left-hand-side of (14) in the thermodynamic limit is quite different. For the diffusive state discussed above  $\delta A(t, \Psi) \sim e^{-t/\tau}$ . Then

$$\int_{-\infty}^{\infty} \delta A(t, \Psi) \frac{\sin(\pi t/T)}{\pi t} dt = \frac{2}{\pi} \arctan\left(\frac{\pi \tau}{T}\right). \quad (17)$$

For large  $T \gg \tau$  this reduces to  $2\tau/T$ , which is in agreement with the approximate expression (7) and the qualitative picture that  $\delta A(t, \Psi)$  remains of order one for the time  $t \sim \tau$  and then can be taken to be zero. When  $T$  is large but not necessarily larger than  $\tau$  (17) remains of order one and the inequality (14) can not be satisfied. For (14) to be satisfied  $T$  has to be parametrically larger than  $\tau$ ,

$$\left(\frac{\tau}{T}\right)^2 \lesssim \frac{\sqrt{t_D \tau}}{T} \Rightarrow T \gtrsim t_D^{-1/2} \tau^{3/2} \sim L^3. \quad (18)$$

It is interesting to note that the scaling  $T \sim L^3$  coincides with the condition that the first and second terms in (8) are of the same order. In other words this is the strongest bound one can consistently obtain from (14) using the state  $|\Psi\rangle$  introduced above. To summarize, we see that the inequality (14) imposes a stringent bound on the energy scale  $\Delta E_{\text{RMT}}$ , which should be parametrically smaller than the Thouless energy  $\Delta E_{\text{Th}} = \tau^{-1}$ . In particular, for the 1D diffusive systems we find

$$\Delta E_{\text{RMT}} \lesssim L^{-3}. \quad (19)$$

For a translationally-invariant system it is also illustrative to consider an operator  $A_k$  with constant momentum. Keeping in mind a 1D spin lattice system of

length  $L$ , we denote by  $A_{(m)}$  a local operator  $A$  located at the site  $m$ . Then

$$A_k = \frac{2^{1/2}}{L^{1/2}} \sum_{m=1}^L \cos(km) A_{(m)}, \quad (20)$$

where  $L$  is dimensionless. The normalization factor  $(2/L)^{1/2}$  is chosen such that the connected autocorrelation function is  $L$ -independent in the thermodynamic limit

$$\langle A_k(t) A_{-k} \rangle_\beta \simeq e^{-k^2 D t}. \quad (21)$$

With the same normalization the expectation value (5) in the diffusive state will be

$$\delta A(t, \Psi) \sim L^{1/2} e^{-k^2 D t} \quad (22)$$

Although the  $t$ -dependence in (21) and (22) is the same, different  $L$ -dependent prefactor will result in a constraint for  $\Delta E_{\text{RMT}}$ . For large  $T \gg 1/(k^2 D)$  we can estimate

$$\int_0^\infty \frac{\sin(\pi t/T)}{\pi t} e^{-k^2 D t} dt \sim \frac{1}{k^2 D T} \quad (23)$$

After ignoring unimportant numerical prefactors (14) yields

$$\frac{L}{k^2 D T} \lesssim 1 \quad \Rightarrow \quad T \gtrsim L/(k^2 D). \quad (24)$$

For fixed  $k$ , the initial configuration with the characteristic wavelength  $1/k$  will require a finite  $L$ -independent time  $1/(k^2 D)$  to thermalize. Thus, we have shown that for  $A_k$  the inverse Random Matrix Theory scale  $\Delta E_{\text{RMT}}^{-1} \gtrsim L/(k^2 D)$  is parametrically longer than the thermalization time.

*Conclusions.* We have shown that the energy scale  $\Delta E_{\text{RMT}}$  at which the ETH ansatz reduces to Random Matrix Theory has to be parametrically smaller than the inverse characteristic time of the slowest mode probed by the corresponding operator  $A$ . For the 1D diffusive system and local operator  $A$  coupled to the diffusive quantity we found  $\Delta E_{\text{RMT}}$  to be bounded by  $L^{-3}$ , where  $L$  is the system size. Our findings suggest that the conventional picture of thermalization of quantum ergodic systems, which assumes universal behavior of local observables at the scales below Thouless energy, is incomplete. In particular, there is an additional scale  $\Delta E_{\text{RMT}}$  relevant for thermalization dynamics.

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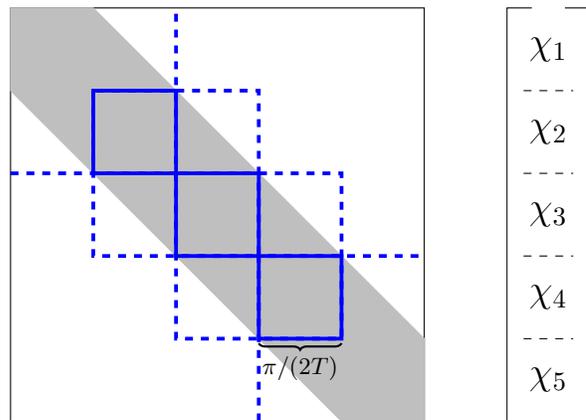


FIG. 1. Schematic visualisation of band matrix  $\delta A_T$  and vector  $|\chi\rangle$  represented as a sum of  $\sum_{I=1}^N |\chi_I\rangle$ .

## APPENDIX

Let us consider a band matrix  $\delta A_T$  such that  $(\delta A_T)_{ij} = 0$  unless  $|E_i - E_j| \leq \pi/T$ , and indices  $i, j$  satisfy (10) for some  $E$  and  $\Delta E$ . The largest eigenvalue of  $(\delta A_T)$  is a monotonically non-decreasing function of  $\Delta E$ . It will be convenient to assume that  $2\Delta E = N\pi/(2T)$  for some integer  $N$ , which can be always achieved by appropriately increasing  $\Delta E$ . Such matrix with  $N = 5$  is schematically shown in Fig. 1, where for the illustrative purposes we assume  $E_i$  are continuous and parametrize matrix elements using unfolded energies  $\mathcal{E}_i$ ,  $d\mathcal{E} = \Omega(E)dE$ . The largest eigenvalue of  $\delta A_T$  can be defined via maximization problem

$$\lambda(\delta A_T) = \max_{\chi} \langle \chi | \delta A_T | \chi \rangle \quad (25)$$

where maximization is over all normlized  $|\chi|^2 = 1$  states  $|\chi\rangle = \sum_i c_i |E_i\rangle$  with  $E_i \in [E - \Delta E, E + \Delta E]$  and otherwise arbitrary  $c_i$ . We would like to introduce  $N$  projectors  $P_I$  acting on  $|\chi\rangle$  as follows

$$|\chi_I\rangle \equiv P_I |\chi\rangle = \sum_{|4(E_i - E)T/\pi + (N+1-2I)| < 1} c_i |E_i\rangle, \quad (26)$$

where  $I = 1 \dots N$ . Clearly  $|\chi\rangle = \sum_{I=1}^N |\chi_I\rangle$ , which is schematically depicted in Fig. 1. We also introduce  $|\chi_{I,I+1}\rangle \equiv |\chi_I\rangle + |\chi_{I+1}\rangle$ . The band structure of  $\delta A_T$  ensures that  $\langle \chi_I | \delta A_T | \chi_J \rangle = 0$  unless  $|I - J| \leq 1$ . Therefore

$$\langle \chi | \delta A_T | \chi \rangle = \sum_{I=1}^{N-1} \langle \chi_{I,I+1} | \delta A_T | \chi_{I,I+1} \rangle - \sum_{I=2}^{N-1} \langle \chi_I | \delta A_T | \chi_I \rangle.$$

The matrix elements above can be bounded by (here  $E''_I$  are the centers of the small blue squares in Fig. 1)

$$|\langle \chi_I | \delta A_T | \chi_I \rangle| \leq |\chi_I|^2 x(E''_I, \pi/(4T), T), \\ E''_I = E + (2I - N - 1)\pi/(4T),$$

and similarly  $\langle \chi_{I,I+1} | \delta A_T | \chi_{I,I+1} \rangle$  is bounded by  $|\chi_{I,I+1}|^2 x(E'_I, \pi/(2T), T)$ , where

$$E'_I = E + (2I - N)\pi/(4T) \quad (27)$$

are the centers of the large blue dashed squares in Fig. 1. We introduce  $E''$  as the value of  $E'_I$  for  $I = 2 \dots N - 1$  for which  $x(E'_I, \pi/(4T), T)$  is maximal, and similarly  $E'$  for  $x(E'_I, \pi/(2T), T)$  and  $I = 1 \dots N - 1$ . As a result we find

$$\langle \chi | \delta A_T | \chi \rangle \leq \sum_{I=1}^{N-1} |\chi_{I,I+1}|^2 x(E', \pi/(2T), T) + \sum_{I=2}^{N-1} |\chi_I|^2 x(E'', \pi/(4T), T). \quad (28)$$

Finally, from

$$\sum_{I=1}^{N-1} |\chi_{I,I+1}|^2 = 2 - |\chi_1|^2 - |\chi_N|^2, \quad (29)$$

$$\sum_{I=2}^{N-1} |\chi_I|^2 = 1 - |\chi_1|^2 - |\chi_N|^2, \quad (30)$$

and (28) we find the bound (11).

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