Phase transition and annealing in quantum random energy models

Carlo Presilla\textsuperscript{1,2,3} and Massimo Ostilli\textsuperscript{4,2}

\textsuperscript{1}Dipartimento di Fisica, Università di Roma “La Sapienza”, Piazzale A. Moro 2, Roma 00185, Italy
\textsuperscript{2}Statistical Mechanics and Complexity, INFN-CNR Research and Development Center, Roma, Italy
\textsuperscript{3}INFN, Sezione di Roma 1, Roma, Italy
\textsuperscript{4}Departamento de Física da Universidade de Aveiro, 3810-193 Aveiro, Portugal

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By using a previously established exact characterization of the ground state of random potential systems in the thermodynamic limit, we determine the ground and first excited energy levels of quantum random energy models, discrete and continuous, and rigorously establish the existence of a first order quantum phase transition. Our analysis, corroborated by Monte Carlo simulations, suggests that the presence of an exponentially vanishing minimal gap at the transition does not prevent the success of a quantum annealing algorithm.

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The perspective to realize a physical device representing a quantum computer (QC) has motivated a fervent research activity concerning the algorithms that could best exploit the intrinsic quantum properties of such a computer as opposed to the classical ones of current computers. In particular, there has been a growing interest toward the possibility to use quantum annealing (QAn) \cite{5–7} as an alternative to simulated thermal annealing \cite{1–3}. A pictorial viewpoint in fact suggests that in order to get the ground state (GS) of a given classical Hamiltonian $V$, the thermal fluctuations, introduced to avoid the system to be trapped in local minima, could be replaced by quantum fluctuations able to outperform the former due to tunneling effects. Usually, QAn is associated with quantum adiabatic (QAd) algorithms \cite{5–7}. The idea is to implement an interpolating Hamiltonian $H(\Gamma) = V + \Gamma K$, where $K$ is an operator which does not commute with $V$. The adiabatic theorem ensures that for sufficiently slow changes of the parameter $\Gamma$ the interpolating system remains in its GS so that the original GS of $V$ can be recovered in the limit $\Gamma \to 0$. However, for many interesting problems $V$ the interpolating Hamiltonian $H(\Gamma)$ is likely to undergo a first order phase transition at some value $\Gamma = \Gamma_c$, where the energy gap $\Delta$ between the first excited state (FES) and the GS becomes exponentially small in the system size $N$ \cite{8,9}. In this case, a QAd decrease of $\Gamma$ starting from some value $\Gamma > \Gamma_c$, where the GS of $H(\Gamma)$ is found with ease, requires an exponentially long time. Otherwise, the system evolves into a combination of several instantaneous eigenstates of $H(\Gamma)$ and when $\Gamma \to 0$ there is a finite probability to attain a state of $V$ different form the GS. For $V$ with a glassy energy landscape, “quantum is better” may be untrue \cite{10}.

We will show that, despite the above pessimistic scenario, a QC could still be used to almost solve the problem of finding the nearly degenerate GS of a classical random problem $V$ by a QAn algorithm running in a time polynomial in the system size $N$. By this we mean the following. For any fixed size $N$, let the problem $V$ represent an ensemble of random systems characterized by a distribution $q_N(\Delta)$ of the energy gap $\Delta$ between GS and FES. Unless $q_N(\Delta)$ takes a Dirac-$\delta$ like contribution in $\Delta = 0$, the fraction of system samples having $\Delta \leq t^{-1}$, namely $f_N(t) = \int_0^{1/t} q_N(\Delta) d\Delta$, vanishes for $t \to \infty$. By performing $k$ annealing steps, each one employing a quantum computation time $t$, and with $k$ growing no more than polynomially in $N$, our algorithm succeeds in finding the GS for a fraction $1 - f_N(t)$ of systems in the ensemble $V$. Note that we don’t know a priori if the system sample considered is one of those for which the GS can be found exactly or not. In any case, however, the error in the found GS energy is $O(t^{-1})$. How fast $f_N(t)$ approaches 0 by increasing $t$ is a notion which could be used to discriminate between simple and hard almost-solvable problems. Below, we discuss two examples. In one $f_N(t) \lesssim q_N(0)t^{-1}$, in the other $f_N(t) = r_N$ constant and the problem is not almost solvable. We have checked these results by Monte Carlo (MC) simulations.

We illustrate our idea in the case in which $V$ is a general random energy model (REM) with discrete or continuous distribution of the levels. For any choice of $K$, provided that $K$ has zero diagonal elements in the representation in which $V$ is diagonal, $H(\Gamma) = V + \Gamma K$ is a quantum random energy model (QREM) belonging to the class of systems studied in \cite{11}. For these systems, we have exactly characterized the GS and found a sufficient condition for the existence of a first order quantum phase transition \cite{11}. Here we extend the results of \cite{11} to study both GS and FES energies of a generic QREM. The REM with a Gaussian distribution is a well known toy model for spin glasses \cite{12} and the corresponding QREM has been first studied perturbatively and numerically in \cite{3}. This model provides an example of an almost solvable problem. The closely related QREM with binomial distribution of levels turns out to be unsolvable.

Ground state of random potential systems. In \cite{11} we have determined the exact GS of a class of Hamiltonian
models defined by a generic hopping operator of dimension $M$ and a potential taking $M$ i.i.d. random values. For this class of models, in the thermodynamic limit the energy $E_0$ of the GS is related to the lowest level $E_0^{(0)}$ of the hopping operator by

$$
\int \frac{P(V)}{E_0 - V} \, dV = \frac{1}{E_0^{(0)}}, \quad E_0 \leq E(V(1)),
$$

where $P(V)$ is the distribution of the random potential values $V$ and $E(V(k))$ is the expectation of the associated $k$-th order statistic \( \text{median} \), i.e. the expectation of the $k$-th smallest value among the $M$ values of $V$ drawn according to $P(V)$. Note that, whereas $E_0^{(0)}$ is deterministic, $E_0$ is random and \( \text{median} \) is an equation for the expectation $E(E_0)$. However, we assume that $E_0$ is zero-averaging which justifies the above notation. The integration interval in \( \text{median} \) corresponds to the support $(V_{\text{min}}, V_{\text{max}})$ of $P(V)$.

If, by changing a parameter below some threshold, e.g. $\Gamma < \Gamma_c$, the solution of the integral equation in \( \text{median} \) becomes incompatible with the constraint $E_0 \leq E(V(1))$, then the GS of the system freezes into that for which $V$ is the minimum occurred value of the given sample and $E_0(\Gamma) = E(V(1))$ for any $\Gamma < \Gamma_c$. A sufficient condition for this first order phase transition to take place is that $P(V) \to 0$ when $V \to V_{\text{min}}$ \( \text{median} \). If $V_{\text{min}} = -\infty$, the normalization of $P(V)$ ensures that this condition is always satisfied.

**Discrete and continuous QREMs.** Let us consider the Hamiltonian $H = \Gamma K + V$ acting on the $M = 2^N$ spin states $|n\rangle = |n_1, n_2, \ldots, n_N\rangle = |n_1\rangle|n_2\rangle \ldots |n_N\rangle$, where $|n_i\rangle$ is eigenstate of the Pauli matrix $\sigma_i^z$, $i = 1, \ldots, N$. The hopping operator $K$ is chosen as the sum of single-flip operators $K = -\sum_{i=1}^{N} \sigma_i^z \otimes \sigma_2^z \otimes \ldots \otimes \sigma_i^z \otimes \ldots \otimes \sigma_N^z \otimes \ldots$, $\sigma_i^z$ being the Pauli matrix acting on the $i$-th spin. More general forms for $K$ can be considered and tackled in a similar way. The potential $V$ is a diagonal operator with elements $V_n = \langle n | V | n \rangle$ i.i.d. random variables drawn with distribution $P(V)$. As an example of discrete QREMs we will consider the case in which $V$ takes the values $V_k = -J(N-2k)$, $k = 0, 1, \ldots, N$, with probability mass function $P(V_k) = 2^{-N(N)}$. We will refer to this model as the binomial QREM. As an example of continuous models we will assume $V \in (-\infty, +\infty)$ with probability density function $P(V) = (\pi N J^2)^{-1/2} \exp(-V^2/(N J^2))$. We will refer to this model as the Gaussian QREM.

In the thermodynamic limit $N \to \infty$, the integral in Eq. \( \text{median} \) can be performed exactly by the saddle-point method. The spectrum of $\Gamma K$ is trivial and, in particular, its GS level is $E_0^{(0)} = -\Gamma N$. Equation \( \text{median} \) thus provides

$$
E_0 = \begin{cases} 
E(V(1)) & \Gamma < \Gamma_c, \\
-\Gamma N & \Gamma \geq \Gamma_c,
\end{cases}
$$

where $\Gamma_c = \lim_{N \to \infty} -E(V(1))/N$. Stated in this form, the result applies to any QREM. In the binomial case $E(V(1)) = -JN + O(1)$, whereas in the Gaussian model $E(V(1)) = -JN \sqrt{\ln 2} + O(1)$. The critical hopping parameter separating the frozen and paramagnetic phases is then $\Gamma_c = J$ and $\Gamma_c = J \sqrt{\ln 2}$, respectively.

By introducing auxiliary Hamiltonians, we can use again Eq. \( \text{median} \) to evaluate excited eigenvalues of $H$. Suppose, at first, that we are in the frozen phase $\Gamma N < -E(V(1))$. For a given realization of the random potential $V$, the GS of $H$ is $|n_1\rangle$, where $|n_k\rangle$ is the configuration of the $k$-th smallest value of the potential, i.e. $V_{n_1} < V_{n_2} < \ldots$. We then introduce the Hamiltonian $H = H - V_{n_1}|n_1\rangle\langle n_1|$ whose lowest eigenvalue $\tilde{E}_0$ coincides with the level $E_1$ of $H$. Note that $\tilde{H}$ describes a system with random potential $V$ having distribution $P(V)$ such that $E(V(1)) = E(V(2))$. Moreover, the operators $\tilde{H}$ and $H$ have the same non-diagonal part, i.e. $\tilde{E}_0^{(0)} = E_0^{(0)}$, so that from \( \text{median} \) we find

$$
\tilde{E}_0 = \begin{cases} 
E(V(2)) & \Gamma < -E(V(2))/N, \\
-\Gamma N & \Gamma \geq -E(V(2))/N.
\end{cases}
$$

We proceed with a similar analysis in the paramagnetic phase. For $\Gamma N \gg -E(V(1))$, the GS of $H$ approaches the GS of $K$, namely $|0_K\rangle = 2^{-N/2} \sum_n |n\rangle$. Observing that $E((0_K|H|0_K\rangle) = -\Gamma N$ exactly for any $\Gamma$, we assume $|0_K\rangle$ to represent an effective GS in all the paramagnetic region. We then introduce the Hamiltonian $\tilde{H} = H + \Gamma N|0_K\rangle\langle 0_K|$, which we guess, has the average lowest eigenvalue $\tilde{E}_0$ coincident with the average level $E_1$ of $H$. Note that $\tilde{H}$ describes a system with random potential $\tilde{V} = V + \Gamma N 2^{-N}$ having distribution $P(\tilde{V}) = P(V)$. The non-diagonal part of $\tilde{H}$ is $\Gamma K + \Gamma N 2^{-N}U$ where $U$ has matrix elements $U_{n,n'} = 1 - \delta_{n,n'}$. It can be shown that any one of the $N$-degenerate FESs of $K$, $\langle 1 | \sigma_i^z | 0_K \rangle$, $i = 1, \ldots, N$, is a GS of $K + N 2^{-N}U$ with eigenvalue $-(N-2)N 2^{-N}$. By inserting $E_0^{(0)} = -\Gamma(N-2)N 2^{-N}$, and $E(V(1)) = E(V(1)) + \Gamma N 2^{-N}$ into Eq. \( \text{median} \), we get

$$
\tilde{E}_0 = \begin{cases} 
E(V(1)) + \Gamma N 2^{-N} & \Gamma < -E(V(1))/N, \\
-\Gamma(N-2)N 2^{-N} & \Gamma \geq -E(V(1))/N.
\end{cases}
$$

Now we combine \( \text{median} \) and \( \text{median} \) to obtain $E_1$. Observing that $\lim_{N \to \infty} (E(V(2)) - E(V(1)))/N = 0$, we conclude that in the thermodynamic limit

$$
E_1 = \begin{cases} 
E(V(2)) & \Gamma < \Gamma_c, \\
-\Gamma(N-2)N 2^{-N} & \Gamma \geq \Gamma_c.
\end{cases}
$$

Equation \( \text{median} \) and hence $E_0$ and $E_1$ found above are exact up to terms $O(1)$ \( \text{median} \). However, the $O(1)$ errors obtained for $E_0$ and $E_1$ match when $N \to \infty$. It follows that for $N \to \infty$ the average gap $E(\Delta) = E_1 - E_0$ is

$$
E(\Delta) = \begin{cases} 
E(V(2)) - E(V(1)) & \Gamma < \Gamma_c, \\
2\Gamma & \Gamma \geq \Gamma_c.
\end{cases}
$$
In the frozen phase, the average gap is a constant which amounts to $E(\Delta)/J = 2/e$ in the binomial case and $E(\Delta)/J \approx 0.6$ in the Gaussian model.

The results of Eqs. (2), (3) and (6) have been compared with those from exact numerical diagonalizations of $H$ for different values of the system size $N$. In Fig. 1 we show the behavior of the average gap in the Gaussian QREM. In both binomial and Gaussian models, the data obtained for $N$ from 8 to 22 exhibit a systematic convergence toward the thermodynamic limit (0).

Our numerical data confirm that, as usually assumed, the extensive quantities $E_0$ and $E_1$ are self-averaging.

For the gap we observe a different behavior. In the paramagnetic phase $\Delta$ is self averaging whereas this property is lost in the frozen phase. In the inset of Fig. 1 we show the frequencies of the gap values at the critical point for the Gaussian QREM. It is evident that $\lim_{N \to \infty} \text{var}(\Delta)/E(\Delta)^2 \neq 0$. The same conclusion is reached for both binomial and Gaussian QREMs in the whole range $0 \leq \Gamma \leq \Gamma_c$.

The gap distributions for the binomial and the Gaussian QREMs have well distinct shapes in the frozen phase. In the discrete model, when $\Gamma$ is decreased below $\Gamma_c$ the gap values concentrate around $\Delta = 0, 2J, 4J, \ldots$. Including only terms not vanishing in the limit $N \to \infty$, at $\Gamma = 0$ the gap distribution becomes

$$q_N(\Delta) \approx q_N(0) \exp[-q_N(0)\Delta],$$

where $q_N(0)$ quickly saturates for $N \to \infty$ to a constant value near $1/(0.6J)$.

Minimal gap and QAd algorithms. To complete the study of the gap, it is useful to define two other quantities $\tilde{\Delta}$ and $\bar{\Delta}$. For any chosen system sample of size $N$, $\Delta(\Gamma)$ has a minimum at $\Gamma = \Gamma_{\text{min}}$, see Fig. 2. Let us define $\Delta_{\text{min}} = \min_{\Gamma \geq 0} \Delta(\Gamma)$. Theoretical arguments, checked numerically for both Gaussian and binomial QREMs, show that $\Delta_{\text{min}}$ and $\Gamma_{\text{min}}$ are self-averaging quantities, whereas for each size $N$ the symbols joined by straight lines are the averages from exact numerical diagonalization of 1000 system samples. Insert: histograms of the frequencies of the gap values evaluated at $\Gamma = \Gamma_c$ (size $8 \leq N \leq 22$ from top to bottom, curves shifted for the sake of clarity).

For later use we also note that for $|\Delta(\Gamma)| \leq c/N$ the superposition of the lowest eigenstates of $H(\Gamma)$, $|\psi(\Gamma)\rangle$ with $\Delta(\Gamma) \approx 0$, provides the analytical estimates

$$\Gamma_{\text{min}} = -V_{n_1}/N$$

and

$$\Delta_{\text{min}} = -2V_{n_1} = 2N^{-2/3}.$$ 

Properties $i)$, $ii)$ and $iii)$ follow straightforwardly from these expressions observing that $V_{n_1} = V(1)$ and $\text{var}(V(1))$ approaches a constant close to $\Gamma_c^2$ for $N \to \infty$.

Note that for $\Gamma < \Gamma_c$, where $\Delta$ is not self-averaging, $E(\Delta)$ loses memory of the sample dependent minimum of the gap, see Fig. 1. On the other hand, the self-averaging property in force for $\Gamma > \Gamma_c$ implies that $E(\Delta) \approx \Delta$ changes smoothly, at finite $N$, between the frozen and the paramagnetic regimes for $\Gamma \in [\Gamma_{\text{min}}, \Gamma_{\text{min}} + \Gamma_c/N]$. For later use we also note that for $|\Gamma - \Gamma_{\text{min}}| \leq c/N$ the superposition of the GS $|\psi_0(\Gamma)\rangle$ with both states $|0_K\rangle$ and $|n_1\rangle$ is much larger than $|0_K|n_1\rangle = 2N^{-2/3}$. In the crude approximation, we have $a_0(\Gamma) \approx 1$ for $\Gamma > \Gamma_{\text{min}}$ and $a_0(\Gamma) \approx 1/[2 + (N(\Gamma - \Gamma_{\text{min}})/2V_{n_1} - 2N^{-2/3})]^{-1}/2$ for $\Gamma < \Gamma_{\text{min}}$. Identical expressions hold for $b_0(\Gamma)$ in the reversed regions $\Gamma < \Gamma_{\text{min}}$ and $\Gamma > \Gamma_{\text{min}}$, respectively. In the Ritz method with a larger superposition of states, $|\psi_0(\Gamma)\rangle$ has for $|\Gamma - \Gamma_{\text{min}}| \leq \Gamma_c/N$ a substantial superposition also with a few of other $V$ eigenstates, namely $|n_2\rangle, |n_3\rangle, \ldots$, and their associated $N$ first neighbors.

Points $i)$ and $ii)$ imply that a QAd algorithm to find $V_{n_1}$ would require a computational time $t > \Delta_{\text{min}}^{-1}$ exponentially long with $N$ for almost any system sample. In principle, one can hope to elude this limitation by using an adiabatic path in which the transit through a gap minimum is avoided. However, it is not clear how to realize this path for $V$ of the class considered here.

**Imaginary time non adiabatic QAn algorithm.** In alternative, consider the following non adiabatic strategy. Chosen a system sample of size $N$, let it to evolve for an imaginary time $s \in [-\infty, 0]$ with the time dependent Hamiltonian $H(\Gamma(s))$, where $\Gamma(s) = \sum_{j=0}^{k} \chi_{j} \Gamma_j \xi_j [j, j+1] \delta(s)$, $\chi_{[a,b]}$ being the characteristic function of the interval $[a, b]$. For simplicity, we set $\Gamma_0 = 0 = j\mathcal{B}$, $j = 1, \ldots, k$, with $\Gamma_k \approx 0$. We also choose $\Gamma_0 \gg \Gamma_{\text{min}}$ so that we
can initialize the system state to the approximate GS of $H(\Gamma_0)$, i.e., $|\psi(0)\rangle = |0\rangle$. If $\delta\Gamma \approx 2\Gamma_0/N$, even if $V_{n_s}$ is unknown, with probability 1 for $N \to \infty$, one of the $\Gamma_j$ values, let say $\Gamma_j$, occurs at time $s = j.t$ in the gap valley of the system sample $[\Gamma_{\text{min}} - \Gamma_c/N, \Gamma_{\text{min}} + \Gamma_c/N]$. At the generic time $s = jt$, when $\Gamma(s)$ suddenly drops from $\Gamma_{j-1}$ to $\Gamma_j$, the system state $|\psi(jt)\rangle$, which has partially relaxed to the GS of $H(\Gamma_{j-1})$, does not change. Nevertheless, rewritten in the basis of the eigenstates of $H(\Gamma_j)$, it is a non trivial superposition which, in the next interval $[jt, jt + t]$, partially relaxes to $|E_0(\Gamma_j)\rangle$. In a formula $|\psi(jt + t)\rangle = \sum_n \langle E_n(\Gamma_j) |\psi(jt)\rangle e^{-E_n(\Gamma_j)t} |E_n(\Gamma_j)\rangle$.

Until $j < j_s$, we have $|E_0(\Gamma_j)\rangle \simeq |0\rangle$ and $|\psi(jt + t)\rangle$ remains close to the GS of $H$. At $j = j_s$, $|E_0(\Gamma_{j_s})\rangle$ has a substantial superposition with both $|0\rangle$ and $|n_1\rangle$. It follows that the probability to find the system at time $j_t + t$ in the GS of $V$, $|\langle n_1 |\psi(j_t + t)\rangle|^2/|\langle \psi(j_t + t)\rangle|^2$, is much larger than the bare value $|\langle n_1|0\rangle|^2 = 2^{-N}$.

As discussed before, transitions into a few of other $\Gamma$ eigenstates, in particular $|n_2\rangle, |n_3\rangle, \ldots$, take place with probabilities of similar order. The evolution steps $j > j_s$, during which $|E_0(\Gamma_j)\rangle \simeq |n_1\rangle$, filter out all these excited eigenstates of $V$, provided that $\Delta(0) = V_{n_2} - V_{n_1} > t^{-1}$. Since $\Delta(0)$ is non self-averaging, it depends on the system sample if this condition does apply or not for a chosen $t$. In the binomial case, the fraction of system samples of size $N$ having $\Delta(0) > t^{-1}$ is $f_N(t) = t_N$, whereas in the Gaussian model $f_N(t) \lesssim q_N(t)/t$. We conclude that for $N$ large the fraction of Gaussian samples for which the QAn algorithm does not succeed vanishes as $t^{-1}$, whereas in the binomial case this fraction is $1 - 1/e$.

We have verified the above scenario by means of MC simulations. The matrix elements of the imaginary time evolution operator $\mathcal{T} \exp(- \int_0^t H(\Gamma(s)) ds)$ obtained by our MC algorithm are exact except for the statistical error caused by the use of a necessarily finite number of random walks in the configuration space. Figure 2 shows the results for one Gaussian QREM sample of size $N = 20$. At the end of each time interval of length $t$, the hopping parameter is decreased stepwise from the value $\Gamma = J$ with $\Delta \Gamma = 0.1J$. For every step we compare the exact GS energy $E_0(\Gamma)$, obtained by numerical diagonalization, with $E_0^{\text{MC}}(\Gamma)$, the GS energy estimated by the MC executing a set of $T$ random walks. In Fig. 2 we also show the gap $\Delta(\Gamma)$ of the system sample under examination. This gap has a minimum $\Delta_{\text{min}} \simeq 0.018J$ at $\Gamma_{\text{min}} \simeq 0.7J$, whereas its value at $\Gamma = 0$ is $\Delta(0) \simeq 0.06J$. For $t = 8/J$, i.e. $\Delta(0) < t^{-1}$, the value of $E_0^{\text{MC}}(\Gamma)$ obtained for $\Gamma \to 0$ may occasionally provide the correct result $E_0(0) = V_{n_1}$, see data for $T = 2^{16}$, but erratic results are produced for different values of $T$. On the other hand, whenever $\Delta(0) > t^{-1}$ a systematic convergence $E_0^{\text{MC}}(\Gamma) \to E_0(0)$ is observed for $\Gamma \to 0$ by increasing $T$. Note that for $T = 32/J$ the error $E_0^{\text{MC}}(\Gamma) - E_0(\Gamma)$ is large near $\Gamma_{\text{min}}$ where $\Delta(\Gamma) < t^{-1}$. For $t = 64/J$, i.e. $\Delta_{\text{min}} > t^{-1}$, a QAd condition is achieved and $E_0^{\text{MC}}(\Gamma)$ is close to $E_0(\Gamma)$ for any value of $\Gamma$.

In the MC implementation of our QAn algorithm the total computation time is proportional to $ktT$. By increasing $N$, provided $\Delta(0) > t^{-1}$, $E_0(0)$ is found if the number of annealing steps scales as $k \sim N$ and the number of random walks as $T \sim 2^N$. Thus the total computation time increases exponentially with the system size $N$. The conclusion would be drastically different by using a QC, say with a number of qubits $\geq N$. In that case, we wouldn’t be in need of a classical probabilistic representation of the matrix elements of $\mathcal{T} \exp(- \int_0^t H(\Gamma(s)) ds)$

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure2.png}
\caption{Relative error in evaluating the GS energy by MC simulations (symbols joined by straight lines, left scale) in a Gaussian QREM sample with $N = 20$ spins. The hopping parameter $\Gamma$ is decreased stepwise from the value $\Gamma = J$ and at each step $E_0^{\text{MC}}(\Gamma)$ is evaluated by executing $T$ random walks in the configuration space for a time $t = 8/J$ (unfilled symbols, $T = 2^{14}, \ldots, 2^{20}$), $t = 32/J$ (filled symbols, $T = 2^{14}, \ldots, 2^{20}$) or $t = 64/J$ (crosses, $T = 2^{14}$). The gap of the system sample $\Delta(\Gamma)$ is also shown (solid line, right scale) in comparison with the chosen $t^{-1}$ values (dashed arrows).}
\end{figure}

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