Localization in the Discrete Non-Linear Schrödinger Equation: mechanism of a First-Order Transition in the Microcanonical Ensemble

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When constrained to high energies, the wave function of the non-linear Schrödinger equation on a lattice becomes localized. We demonstrate here that localization occurs as a first-order transition in the microcanonical ensemble, in a region of phase space where the canonical and the microcanonical ensembles are not equivalent. Quite remarkably, the transition to the localized non-ergodic phase takes place in a region where the microcanonical entropy, $S_N$, grows sub-extensively with the system size $N$, namely $S_N \sim N^{1/3}$. This peculiar feature signals a shrinking of the phase space and exemplifies quite a typical scenario of "broken ergodicity" phases. In particular, the localized phase is characterized by a condensation phenomenon, where a finite fraction of the total energy is localized on a few lattice sites. The detailed study of $S_N(E)$ close to the transition value of the energy, $E_c$, reveals that its first-order derivative, $\frac{dS_N(E)}{dE}|_{E=E_c}$, exhibits a jump, thus naturally accounting for a first-order phase transition from a thermalized phase to a localized one, which is properly assessed by studying the participation ratio of the site energy as an order parameter. Moreover, we show that $S_N$ predicts the existence of genuine negative temperatures in the localized phase. In a physical perspective this indicates that by adding energy to the system it condensates into increasingly ordered states.
I. INTRODUCTION

Beyond its phenomenological interest for many physical applications, such as Bose-Einstein condensates in optical lattices [1, 2] or light propagating in arrays of optical waveguides [3], in the last decades the Discrete Nonlinear Schrödinger Equation (DNLSE) has revealed an extremely fruitful testbed for many basic aspects concerning statistics and dynamics in Hamiltonian models, equipped with additional conserved quantities, other than energy (e.g., see [5] and [6]). In particular, since the pioneering paper by Rasmussen et al. [7], the existence of a high-energy phase characterized by the condensation of energy in the form of breathers, i.e. localized nonlinear excitations, has attracted the attention of many scholars. The phase diagram shown in Fig. 1 summarizes the scenario described in [7]. From a dynamical point of view, extended numerical investigations have pointed out that in such a phase the Hamiltonian evolution of an isolated chain exhibits long-living multi-breather states, that last over astronomical times [2, 3]. Moreover, time averages of suitable non-local quantities entering the definition of temperature \( T \), as, e.g., the inverse of the derivative of the microcanonical entropy \( S \) with respect to the energy \( E \) (in formulae \( \beta = 1/T = \frac{\partial S}{\partial E} \) [8], predict that \( T \) is negative in this high-energy phase [9]. Relying upon thermodynamic considerations Rumpf and Newell [10] and later Rumpf [11,12] argued that these dynamical states should eventually collapse onto an ”equilibrium state”, characterized by an extensive background at infinite temperature with a superimposed localized breather, containing the excess of energy initially stored in the system. This argument seems plausible in the light of a grand-canonical description, where entropy has to be maximal at thermodynamic equilibrium, in the presence of fluctuations due to heat exchanges with a thermal reservoir. Accordingly, in this perspective long-living multi-breather states were interpreted as metastable ones, thus yielding the conclusion that negative temperature states are not genuine equilibrium ones. Due to the practical difficulty of observing the eventual collapse to the equilibrium state predicted by Rumpf even in lattices made of a few tens of sites, some authors have substituted the Hamiltonian dynamics with a stochastic evolution rule, that conserves energy and particle densities. In this framework the breather condensation phenomenon onto a single giant breather emerges as a coarsening process ruled by predictable scaling properties [15, 16].

Despite many of the dynamical aspects of the deterministic and stochastic evolutions of the DNLSE have been satisfactorily described and understood, still the thermodynamic interpretation of this model remains unclear, because it seems to depend on the choice of the adopted statistical ensemble. In fact, already in [7] the authors point out that an approach based on the canonical ensemble yields a negative temperature in the high-energy phase, which contradicts
the very existence of a Gibbsian measure. Moreover, they claim that only by introducing a suitable grand-canonical representation, at the price of transforming the original short-range Hamiltonian model into a long-range one, allows for a consistent definition of negative temperatures. Also Rumpf makes use of a grand-canonical ensemble to tackle this question [13, 14] and reaches the opposite conclusion that negative temperature states are not compatible with thermodynamic equilibrium conditions. More recently, the statistical mechanics of the disordered DNLSE Hamiltonian has been analyzed making use of the grand-canonical formalism [17]: the authors conclude that for weak disorder the phase diagram looks like the one of the non-disordered model, while correctly pointing out that their results apply to the microcanonical case, whenever the equivalence between ensembles can be established. In a more recent paper the thermodynamics of the DNLSE Hamiltonian and of its quantum counterpart, the Bose-Hubbard model, has been analyzed in the canonical ensemble [21]: the authors even claim that "... the Gibbs canonical ensemble is, conceptually, the most convenient one to study this problem" and conclude that the high-energy phase is characterized by the presence of non-Gibbs states, that cannot be converted into standard Gibbs states by introducing negative temperatures. The main consideration emerging from the overall scenario is that, while in the low-energy phase the thermodynamics of the DNLSE model exhibits standard properties that are consistent with any statistical ensemble representation, in the high-energy phase the very equivalence between statistical ensembles is at least questionable and it cannot be ruled out as a matter of taste.

In this paper we present a clear scenario about the statistical mechanics of the DNLSE problem by performing explicit analytic calculations for the microcanonical ensemble in the high energy limit and, in particular, close to the \( \beta = 0 \) line (see Fig. 1). We want to point out that the thermodynamics of this model is well-defined over the whole phase diagram only in the microcanonical ensemble. In particular, we show explicitly why and how the non-equivalence between statistical ensembles naturally emerges as a manifest consequence of the non-analytic structure of the microcanonical partition function in the high-energy phase. In fact, the large-deviation approach allows us to obtain an explicit analytic expression of the normalized distribution function associated to the microcanonical measure. Moreover, we obtain that the \( \beta = 0 \) line corresponds to a first-order phase transition boundary between a standard extensive phase at low energies and a localized (or condensed) phase at high energies, while including explicit predictions about the scaling of the partition function and finite size corrections. We obtain also the explicit form of the microcanonical entropy and we analyze the transition by computing the participation ratio of the energy per lattice site as the appropriate order-parameter of the first-order phase transition. Finally, we show that, in the natural microcanonical representation, temperatures in the localized phase are truly negative: this is just a consequence of the entropy calculation in the microcanonical ensemble. On the other hand, due to ensemble in-equivalence, this has no counterpart in the canonical and grand-canonical ensembles: any attempt to plug by hand \( T < 0 \) in the canonical/grand-canonical partition function leads unavoidably to some controversy/ambiguity, for the simple reason that it cannot be done. This notwithstanding, numerical simulations performed in [22] show that extended negative temperature regions can be observed also when a sufficiently high thermal gradient is applied by two thermal reservoirs at positive temperatures, coupled to the opposite ends of the DNLSE chain. This tells us that in out-of-equilibrium conditions, the standard thermal phase and the localized one coexist, thus confirming that the microcanonical approach is consistent with the physics contained in the DNLSE model.

This paper is organized as follows. In Sec. II we briefly comment the state of the art of the DNLSE thermodynamics, mainly by the results of Ref. [7]. We introduce also the main object of this study: the microcanonical partition function of the DNLSE, discussing the only approximation done through the whole paper, i.e. the neglecting of the hopping terms, close to the region at infinite temperature. In Sec. III we show how to cast the calculation of the microcanonical partition function as a large deviation calculation, i.e. as the calculation of the probability distribution of independent identically distributed random variables. In particular we show how to account for the non-analytic contribution to the microcanonical partition function, coming from a cut in the negative real semiaxis in the complex \( \beta \) domain of the canonical partition function. Then in Sec. IV we explain how the non-analytic contribution to the partition function gives rise to a discontinuity of the first derivative of the microcanonical entropy and we also compute the order parameter of the transition, the participation ratio. Moreover, we explain how negative temperatures arise naturally in this context and finally, in Sec. V we turn to conclusions. The technical details of the calculations are left for the appendices.
II. THE NON-LINEAR DISCRETIZED SCHRÖDINGER EQUATION: GENERALITIES

In this paper we study the one-dimensional DNLSE, namely a scalar complex field $z_j$ on a one dimensional lattice with periodic boundary conditions made of $N$ sites, whose Hamiltonian reads:

$$
\mathcal{H} = \sum_{j=1}^{N} (z_j^* z_{j+1} + z_j z_{j+1}^*) + \sum_{j=1}^{N} |z_j|^4.
$$

The corresponding Hamiltonian dynamics is expressed by the equations of motion

$$
i \dot{z}_j = -\frac{\partial \mathcal{H}}{\partial z_j^*} = -(z_{j+1} + z_{j-1}) - 2|z_j|^2 z_j.
$$

For what follows, it is crucial to point out that these equations of motion conserve not only the total energy $\mathcal{H}$, but, due to the quantum origin of the problem, also the squared norm of the “wave-function”, that is

$$A = \sum_{j=1}^{N} |z_j|^2.
$$

This functional can be read also as the total number of particles contained in the model. We attribute to $\mathcal{H}$ and $A$ the real values $E$ and $A$, respectively. Due to the presence of these two conserved quantities the deterministic dynamics of this model exhibits quite peculiar features. The overall scenario is summarized in the phase diagram shown in Fig. 1, where $e = E/N$ and $a = A/N$: there is a region contained in between the zero temperature line ($\beta = 1/T = +\infty$) and the infinite temperature one ($\beta = 0$), where any initial condition evolves to a standard thermodynamic equilibrium state, while above the ($\beta = 0$)-line the dynamics of any finite lattice is characterized by the birth and death of long-living localized nonlinear excitations, called breathers (e.g., see [1, 2]). When a stochastic version of the dynamics, still conserving both $E$ and $A$, has been considered [15, 16], the evolution in the region above the ($\beta = 0$)-line has been found to amount to a coarsening process eventually yielding a state where a giant breather confined in a finite lattice region collects a finite fraction of the total energy and norm. In particular, the condensate “mass” has been found to increase in time $t$ as $t^{1/3}$. One cannot exclude that also the deterministic dynamics in the high energy localized phase might eventually evolve to this single-breather state, although it is a matter of fact that it has never been observed, even in relatively small lattices. Finding an interpretation of this...
scenario is related to the understanding of the thermodynamics of the DNLSE model. In fact, various attempts have been made to study its equilibrium properties in the presence of a localized wave-function [7,17]. The reason why a study of the thermodynamics deep in the localized phase has been (to some extent) so far elusive is that the \((\beta = 0)\)-line, where condensation takes place, corresponds also to the breakdown of the equivalence between statistical ensembles, as we are going to show. It is worth at this point to quote a serie of recent papers, focused on the regression dynamics of large anomalous fluctuations, which also had in the background the idea that isolated anomalous fluctuations must be somehow related to ensemble inequivalence [18–20]. Nevertheless, the first demonstration that the physics of a localized phase, which can be indeed seen as an anomalous density fluctuation, finds a fully consistent description only in the microcanonical ensemble, it is a fully original contribution of the present work.

The main goal of this paper amounts to compute the microcanonical entropy of the DNLSE Hamiltonian [Eq. (1)] for fixed values of \(E\) and \(A\) close to the \((\beta = 0)\)-line, shown in Fig. 1. In general, the microcanonical entropy is defined as

\[ S_N(A, E) = \log \Omega_N^O(A, E), \]

where the Boltzmann constant \(k_B\) is set to unit and \(\Omega_N^O(A, E)\) is the microcanonical partition function:

\[ \Omega_N^O(A, E) = \int \prod_{j=1}^N d\mu(z_j) \delta \left( A - \sum_{j=1}^N |z_j|^2 \right) \delta \left( E - \sum_{j=1}^N (z_j^* z_{j+1} + z_i z_{i+1}^*) + \sum_{i=1}^N |z_j|^4 \right). \]

Here \(d\mu(z_j)\) is a shorthand notation for \(d\Re(z_j) \ d\Im(z_j)\). Since the main interesting features of the DNLSE model occur in the vicinity of the \((\beta = 0)\)-line, we can assume that in such conditions the contribution to the total energy \(E\) of the bi-linear hopping term in Eq. (1) can be neglected with respect to the local nonlinear term. Let us fix for instance the specific energy to the value \(e = E/N\), and chose a rescaling of the variables \(z_i\) as to have the local energy always of order \(\mathcal{O}(1)\), i.e., we use \(\hat{z}_i = z_i/e^{1/4}\). In terms of the new variables the Hamiltonian reads:

\[ \mathcal{H} = \sqrt{e} \sum_{j=1}^N (\hat{z}_j \hat{z}_{j+1} + \hat{z}_i \hat{z}_{i+1}) + e \sum_{i=1}^N |\hat{z}_j|^4. \]

Clearly, in the limit of large \(e\) the hopping term is subleading with respect to the local quartic self-interaction and can be neglected, allowing us to write the microcanonical partition function as follows:

\[ \Omega_N(A, E) = \int \prod_{i=1}^N d\mu(z_j) \delta \left( A - \sum_{j=1}^N |z_j|^2 \right) \delta \left( E - \sum_{j=1}^N |z_j|^4 \right). \]

This approximation is not only proper, but even exact in the large-\(N\) limit, as shown by the fact that the very equation \(e = 2a^2\) identifying the \((\beta = 0)\)-line in Fig. 1 (i.e., the boundary of the region for ensemble equivalence) is obtained either by retaining the hopping term in the transfer matrix calculation of [7] or by dropping it, within the saddle-point approximation adopted here in Sec. IV A to estimate the integral in Eq. (5).

We note that \(N\)-fold integrals with two global constraints, as in Eq. (7), appeared also in different contexts. For instance, in Refs. [26–28], such a kind of integrals describe a generalization of mass conservation models, previously studied in [23,25].

**III. THE MICROCANONICAL PARTITION FUNCTION**

In this Section we report explicit calculations of the approximated microcanonical partition function \(\Omega_N(A, E)\) by exploiting a large-deviation technique.

**A. From statistical mechanics to large deviations**

In order to compute \(\Omega_N(A, E)\) it is convenient to express the variables in their polar form \(z_j = \rho_j e^{i\phi_j}\), thus making straightforward the integration over the angular coordinates \(\phi_j\):

\[ \Omega_N(A, E) = (2\pi)^N \int_0^\infty \left[ \prod_{j=1}^N d\rho_j \right] \delta \left( A - \sum_{j=1}^N \rho_j^2 \right) \delta \left( E - \sum_{j=1}^N \rho_j^4 \right). \]
The effective strategy for proceeding in this analytic calculation amounts to releasing the conservation constraint on $A$ by means of a Laplace transform:

$$\tilde{\Omega}_N(\lambda, E) = \int_0^\infty dA \ e^{-\lambda A} \ \Omega_N(A, E) = (2\pi)^N \int_0^\infty \left[ \prod_{j=1}^N d\rho_j \right] \ e^{-\lambda \sum_{j=1}^N \rho_j^2} \ \delta \left( E - \sum_{j=1}^N \rho_j^2 \right). \tag{9}$$

From Eq. (9) the partition function at fixed $A$ can be then obtained by a simple inversion of the Laplace transform:

$$\Omega_N(A, E) = \frac{1}{2\pi i} \int_{\lambda_0 - i\infty}^{\lambda_0 + i\infty} d\lambda \ e^{\lambda A} \ \tilde{\Omega}_N(\lambda, E), \tag{10}$$

where integration goes over a Bromwich contour in the complex $\lambda$ plane. Let us further elaborate Eq. (9) by introducing the change of variables $\rho_j^2 = \varepsilon_j$, thus yielding the new expression

$$\tilde{\Omega}_N(\lambda, E) = \left( \frac{\pi}{2} \right)^N \int_0^\infty \prod_{j=1}^N d\varepsilon_j \ e^{-\lambda \sum_{j=1}^N \sqrt{\varepsilon_j}} \ \delta \left( E - \sum_{j=1}^N \varepsilon_j \right). \tag{11}$$

We can introduce the normalized probability distribution

$$f_\lambda(\varepsilon) = \Theta(\varepsilon) \ \frac{\lambda}{2} \ \sqrt{\varepsilon} \ \exp \left( -\lambda \sqrt{\varepsilon} \right), \tag{12}$$

where $\Theta(\varepsilon)$ is the Heavyside distribution, and rewrite

$$\tilde{\Omega}_N(\lambda, E) = \left( \frac{\pi}{\lambda} \right)^N \ Z_N(\lambda, E) \tag{13}$$

with

$$Z_N(\lambda, E) = \int_0^\infty \prod_{j=1}^N d\varepsilon_j \ f_\lambda(\varepsilon_j) \ \delta \left( E - \sum_{j=1}^N \varepsilon_j \right). \tag{14}$$

Written in this form, the calculation of $Z_N(\lambda, E)$ amounts to computing the probability distribution of the sum of $N$ i.i.d. random variables $\varepsilon_j$, individually described by $f_\lambda(\varepsilon_j)$ and constrained to obey the condition $E = \sum_{j=1}^N \varepsilon_j$. It is well known from the theory of large deviations [25] that this kind of global constraint on the sum of i.i.d. random variables yields a condensation phenomenon, when the individual probability distribution is fat-tailed, i.e. it fulfills the bounds

$$\exp(-\varepsilon) < f_\lambda(\varepsilon) < \frac{1}{\varepsilon^{\gamma}}. \tag{15}$$

According to Eq. (12), this is precisely the case of the partition function $Z_N(\lambda, E)$. In particular, the condensation phenomenon occurs when the total energy $E$ overtakes a threshold value $E_{th}$, that is equal to the average total energy, in formulae

$$E > E_{th} = N \langle \varepsilon \rangle, \tag{16}$$

where the average $\langle \cdot \rangle$ is over the probability distribution $f_\lambda(\varepsilon)$. In the localized phase it is more convenient for the system to condensate the excess energy $\Delta E = E - E_{th}$ (i.e., a macroscopic portion of the total energy) onto a finite region of the lattice. As clearly explained first in [23, 24], localization simply amounts to the fact that for sufficiently large values of $E$ the behaviour of $Z_N(\lambda, E)$ is dominated by the probability distribution $f_\lambda(\varepsilon_1)$ of the single variable. The large-deviation procedure yielding these results is going to be sketched in the following subsection.

We observe that the integral in Eq. (14), i.e. the sum of $N$ i.i.d. random variables, each one obeying a stretched exponential distribution, emerged quite recently in a completely different context. While the existence of a condensation transition with such a stretched exponential distribution was already known before [25, 27], the precise large deviation form of the distribution of the sum was studied only recently by the two of us in [29], by analyzing the $N$-steps cumulative position distribution for a run-and-tumble particle in one dimension. Moreover, in Ref. [29], an
We conclude this subsection by reporting the values of first two momenta and of the variance of the probability distribution in Eq. (12):

\[ \langle \varepsilon \rangle = \frac{2}{\lambda^2} \]
\[ \langle \varepsilon^2 \rangle = \frac{24}{\lambda^4} \]
\[ \sigma^2 = \langle \varepsilon^2 \rangle - \langle \varepsilon \rangle^2 = \frac{20}{\lambda^4} \]  

(17)

It is then worth anticipating the result of the saddle-point calculation in Eq. (51), from which we obtain \( \langle \varepsilon \rangle = 2a^2 \). This, in turn, allows us to point out that the condition \( E = E_{\text{th}} \) in the \((a, \varepsilon)\)-plane of Fig. 1 coincides with the equation identifying the \((\beta = 0)\)-line, i.e.

\[ E = E_{\text{th}} \longleftrightarrow e = \langle \varepsilon \rangle = 2a^2 \]  

(18)

### B. The peculiar analytic properties of the partition function

In order to proceed in the calculation of the partition function \( Z_N(\lambda, E) \) defined in Eq. (14), we can first perform its Laplace transform with respect to \( E \), introducing then its conjugate variable \( \beta \), which is in general a complex number, i.e. \( \beta \in \mathbb{C} \):
\[ \hat{Z}_N(\lambda, \beta) = \int_0^\infty dE \ e^{-\beta E} \ Z_N(\lambda, E) = \int_0^\infty d\varepsilon_1 \ldots d\varepsilon_N \ e^{-\beta \sum_{j=1}^N \varepsilon_j} \prod_{j=1}^N f_\lambda(\varepsilon_j) \]
\[ = \left[ \int_0^\infty d\varepsilon \ e^{-\beta \varepsilon} \ f_\lambda(\varepsilon) \right]^N = \exp \left\{ N \log[z(\lambda, \beta)] \right\} , \tag{19} \]

where
\[ z(\lambda, \beta) = \int_0^\infty d\varepsilon \ e^{-\beta \varepsilon} \ f_\lambda(\varepsilon) = \sqrt{\pi} \frac{\lambda}{2\sqrt{\beta}} \exp \left( \frac{\lambda^2}{4\beta} \right) \text{Erfc} \left( \frac{\lambda}{2\sqrt{\beta}} \right) , \tag{20} \]

and
\[ \text{Erfc} \left( \frac{\lambda}{2\sqrt{\beta}} \right) = \frac{2}{\sqrt{\pi}} \int_{\lambda/(2\sqrt{\beta})}^\infty e^{-t^2} dt , \tag{21} \]

is the complementary error function defined in the complex \( \beta \) plane, with a branch-cut on the negative real semiaxis, see Fig.2. The original microcanonical partition function \( Z_N(\lambda, E) \) can be then recovered by computing the inverse Laplace transform of \( \hat{Z}_N(\lambda, \beta) \):
\[ Z_N(\lambda, E) = \int_{\beta_0-i\infty}^{\beta_0+i\infty} d\beta \ \exp \left\{ \beta E + N \log[z(\lambda, \beta)] \right\} . \tag{22} \]

The integral in Eq. (22) should be evaluated by means of a saddle-point approximation, where \( \beta_0 \) is the real positive solution of the following equation:
\[ \frac{E}{N} = -\frac{1}{z(\lambda, \beta)} \frac{\partial z(\lambda, \beta)}{\partial \beta} , \tag{23} \]

If such a real positive value \( \beta_0 \) exists, it can be physically interpreted as an inverse temperature and one could finally write
\[ \hat{Z}_N(\lambda, E) \approx e^{\beta_0 E + N \log[z(\lambda, \beta_0)]} . \tag{24} \]

What happens in the DNLSE model is that Eq. (23) for \( E < E_{th} \) admits a unique real positive solution and the integration contour is shown by the dashed (blue) line in Fig.2. Conversely, for \( E > E_{th} \) a real positive solution of Eq. (23) does not exist, due to the presence of the branch-cut of \( z(\lambda, \beta) \) on the real negative semiaxis. As a consequence, the calculation of \( Z_N(\lambda, E) \) can be performed by considering the analytic continuation of \( z(\lambda, \beta) \) in the complex \( \beta \) plane and deforming the integration contour as shown by the continuous (red) line in Fig. 2. Following very similar large-deviation calculations, contained in a series of papers \[23, 24, 26, 29\], one can recover \( Z_N(\lambda, E) \) for \( E > E_{th} \), making use of suitable expansions of \( z(\lambda, \beta) \) around the origin \( \beta = 0 \). In order to evaluate \( Z_N(\lambda, E) \) for a given fixed scale \( \Delta E = E - E_{th} \sim N^\gamma \) of the excess energy one needs to retain the leading terms only up to a given scale in the expansion of \( z(\lambda, \beta) \). For instance, as explicitly reported in \[29\], one can evaluate \( Z_N(\lambda, E) \) at the energy scale \( \Delta E = E - E_{th} \sim N^{1/2} \) (Gaussian regime) by expanding \( z(\lambda, \beta) \) around \( \beta = 0 \) up to the order \( \beta \sim N^{-1/2} \), thus obtaining the almost trivial result
\[ Z_N(\lambda, E) = \frac{1}{\sigma \sqrt{2\pi N}} \exp \left[ -\frac{(E - E_{th})^2}{2\sigma^2 N} \right] , \tag{25} \]

which is a straightforward consequence of the Central Limit Theorem, the dependence on \( \lambda \) coming through \( \sigma \) (see Eq. (17)). On the other hand, if one aims at evaluating \( Z_N(\lambda, E) \) at the order \( \Delta E = E - E_{th} \sim N \), which in \[29\] is denoted as the extreme large deviations regime, one has to retain consistently terms of the expansion of \( z(\lambda, \beta) \) up to the order \( \beta \sim 1/N \). In this case one obtains:
\[ Z_N(\lambda, E) \sim \exp \left( -\sqrt{E - E_{th}} \right) . \tag{26} \]

As discussed in Sec. [V.B], the Gaussian regime and the extreme large deviations regime correspond to a delocalized and to a localized phase, respectively. Therefore, in order to understand whether the crossover between these two
phases occurs as a real thermodynamic phase transition, one has to identify an intermediate matching regime, which can be heuristically singled out by the following condition

$$\frac{(E - E_{th})^2}{2\sigma^2 N} \approx \sqrt{E - E_{th}}, \quad (27)$$

allowing to recognize the intermediate scale

$$E - E_{th} \sim N^{2/3}. \quad (28)$$

### C. Matching regime: the non-analytic contribution

The main result of this section is the proof that in the matching regime the partition function splits into the sum of a Gaussian contribution and of an non-analytic one, denoted as $\mathcal{C}(\lambda, \zeta)$:

$$Z_N(\lambda, E) = \frac{1}{\sigma \sqrt{2\pi N}} \exp \left( -N^{1/3} \frac{\zeta^2}{2\sigma^2} \right) + \mathcal{C}(\lambda, \zeta), \quad (29)$$

where

$$\zeta = \frac{E - E_{th}}{N^{2/3}} \quad (30)$$

is a suitable scaling variable essentially inspired by the matching condition in Eq. (27). The first term on the r.h.s. of Eq. (29) comes from the straight part of the deformed contour in Fig. 2 (continuous red line), while the non-analytic contribution, $\mathcal{C}(\lambda, \zeta)$, is due to the non-analyticity at the branch-cut along the negative real axis.

Since for $E > E_{th}$ the saddle-point condition in Eq. (23) has no real solution, we have to consider the analytic prolongation of $z(\lambda, \beta)$ in the complex $\beta$ plane and to evaluate its expansion around the origin $\beta = 0$ separately along the upper and lower branch cut, i.e. for $\Re(\beta) < 0$:

$$\lim_{\delta \to 0} z(\lambda, \beta + i\delta) = z(\lambda, \beta + i0^+)$$
$$\lim_{\delta \to 0} z(\lambda, \beta - i\delta) = z(\lambda, \beta + i0^-). \quad (31)$$

The expansion around $\beta = 0$ yields the expressions

$$z(\lambda, \beta + i0^+) = 1 - \langle \epsilon \rangle \beta + \frac{1}{2} \langle \epsilon \rangle^2 \beta^2 + \ldots + \sqrt{\frac{2\pi}{\langle \epsilon \rangle \beta}} \exp \left( \frac{1}{2 \langle \epsilon \rangle \beta} \right)$$
$$z(\lambda, \beta + i0^-) = 1 - \langle \epsilon \rangle \beta + \frac{1}{2} \langle \epsilon \rangle^2 \beta^2, \quad (32)$$

where $\langle \epsilon \rangle$ and $\langle \epsilon^2 \rangle$ are defined in Eq. (17) in terms of $\lambda$. Accordingly, the expansion of the local free energy reads:

$$\log[z(\lambda, \beta + i0^+)] = -\langle \epsilon \rangle \beta + \frac{1}{2} \sigma^2 \beta^2 + O(\beta^2) + \ldots + \sqrt{\frac{2\pi}{\langle \epsilon \rangle \beta}} \exp \left( \frac{1}{2 \langle \epsilon \rangle \beta} \right)$$
$$\log[z(\lambda, \beta + i0^-)] = -\langle \epsilon \rangle \beta + \frac{1}{2} \sigma^2 \beta^2 + O(\beta^2), \quad (33)$$

where $\sigma$ is defined in Eq. (17) in terms of $\lambda$. The non-analiticity of $z(\lambda, \beta)$ at the cut, clearly expressed by the difference between the first and the second line of Eq. (33), suggests to evaluate the contour integral which defines $Z_N(\lambda, E)$ [see Eq. (22)], by splitting it in two parts:

$$Z_N(\lambda, E) = T^{(+)}(\lambda, E) + T^{(-)}(\lambda, E). \quad (34)$$
The two terms $I^{(+)}(\lambda, E)$ and $I^{(-)}(\lambda, E)$ in the equation above can be evaluated by introducing explicitly the expansions of Eq. (33) into the integral of Eq. (22). Recalling then that $E_{\text{th}} = N(\varepsilon)$ one gets:

$$
I^{(+)}(\lambda, E) = \int_{\Gamma^{(+)}} \frac{d\beta}{2\pi i} \exp \left\{ \beta (E - E_{\text{th}}) + \frac{N}{2} \sigma^2 \beta^2 + N\text{O}(\beta^2) \right\}
$$

$$
I^{(-)}(\lambda, E) = \int_{\Gamma^{(-)}} \frac{d\beta}{2\pi i} \exp \left\{ \beta (E - E_{\text{th}}) + \frac{N}{2} \sigma^2 \beta^2 + N\text{O}(\beta^2) \right\},
$$

(35)

where the integration paths $\Gamma^{(+)}$ and $\Gamma^{(-)}$ are those shown in Fig. 2. A better interpretation of this result can be obtained by introducing the scaling variable $\zeta$ defined in Eq. (30):

$$
I^{(+)}(\lambda, \zeta) = \int_{\Gamma^{(+)}} \frac{d\beta}{2\pi i} \exp \left\{ \beta \zeta N^{2/3} + \frac{N}{2} \sigma^2 \beta^2 + N\text{O}(\beta^3) \right\}
$$

$$
I^{(-)}(\lambda, \zeta) = \int_{\Gamma^{(-)}} \frac{d\beta}{2\pi i} \exp \left\{ \beta \zeta N^{2/3} + \frac{N}{2} \sigma^2 \beta^2 + N\text{O}(\beta^3) \right\}.
$$

(36)

Since $\Re(\beta) < 0$, for asymptotically small values of $\beta$ one has that the non-analytic term $\exp[1/(2(\varepsilon)\beta)]$ is exponentially small and, at leading order in $N$, we can write

$$
\exp \left[ N \sqrt{\frac{2\pi}{\langle \varepsilon \rangle \beta}} \exp \left( \frac{1}{2(\varepsilon)\beta} \right) \right] \approx 1 + N \sqrt{\frac{2\pi}{\langle \varepsilon \rangle \beta}} \exp \left( \frac{1}{2(\varepsilon)\beta} \right).
$$

(37)

By substituting the above expansion into the integral $I^{(+)}(\lambda, \zeta)$ we obtain

$$
I^{(+)}(\lambda, \zeta) = \int_{\Gamma^{(+)}} \frac{d\beta}{2\pi i} e^{\beta \zeta N^{2/3} + \frac{N}{2} \sigma^2 \beta^2 + N\text{O}(\beta^3)} +
$$

$$
+ N \sqrt{\frac{2\pi}{\langle \varepsilon \rangle \beta}} \int_{\Gamma^{(+)}} \frac{d\beta}{2\pi i} \exp \left\{ \beta \zeta N^{2/3} + \frac{N}{2} \sigma^2 \beta^2 + N\text{O}(\beta^3) + \frac{1}{2(\varepsilon)\beta} \right\}.
$$

(38)

Taking inspiration from (29) we adopt the following scaling ansatz for $\beta$

$$
\beta \rightarrow \beta / N^{1/3},
$$

(39)

which is consistent with the idea that in the matching regime the analytic and non-analytic contributions are of the same order, i.e.

$$
\beta \zeta N^{2/3} + \frac{N}{2} \sigma^2 \beta^2 \approx \frac{1}{2(\varepsilon)\beta}.
$$

(40)

Hence, the leading contribution to the integral in Eq. (38) reads

$$
I^{(+)}(\lambda, \zeta) = \frac{1}{N^{1/3}} \int_{\Gamma^{(+)}} \frac{d\beta}{2\pi i} e^{N^{1/3}\beta \zeta + \frac{N}{2} \sigma^2 \beta^2} +
$$

$$
+ N \sqrt{\frac{2\pi}{\langle \varepsilon \rangle \beta}} \int_{\Gamma^{(+)}} \frac{d\beta}{2\pi i} \frac{1}{\sqrt{N^{1/3}\beta}} \exp \left\{ N^{1/3} \left[ \beta \zeta + \frac{N}{2} \sigma^2 \beta^2 + \frac{1}{2(\varepsilon)\beta} \right] \right\}.
$$

(41)

Similarly, the integral in the negative imaginary semiplane has the expression

$$
I^{(-)}(\lambda, \zeta) = \frac{1}{N^{1/3}} \int_{\Gamma^{(-)}} \frac{d\beta}{2\pi i} e^{N^{1/3}\beta \zeta + \frac{N}{2} \sigma^2 \beta^2}.
$$

(42)

By summing these two contributions one finally obtains

$$
Z_N(\lambda, \zeta) = I^{(+)}(\lambda, \zeta) + I^{(-)}(\lambda, \zeta) =
$$

$$
= \frac{1}{N^{1/3}} \int_{-\infty}^{\infty} \frac{d\beta}{2\pi i} e^{N^{1/3}\beta \zeta + \frac{N}{2} \sigma^2 \beta^2} + C(\lambda, \zeta),
$$

$$
= \frac{1}{\sigma \sqrt{2\pi N}} e^{-N^{1/3} \frac{\beta^2}{\sigma^2}} + C(\lambda, \zeta)
$$

(43)
where the non-analytic contribution to the partition function is

\[ C(\lambda, \zeta) = N \sqrt{\frac{2\pi}{\langle \epsilon \rangle}} \int_{\Gamma(\beta)}^{\beta} \frac{d\beta}{2\pi i} \frac{1}{\sqrt{N^{1/3} \beta}} e^{N^{1/3} F(\lambda, \beta)}, \]  

(44)

with

\[ F(\lambda, \beta) = \beta \zeta + \frac{1}{2} \sigma^2 \beta^2 + \frac{1}{2} \frac{1}{\langle \epsilon \rangle} \beta. \]  

(45)

The decomposition of the partition function in the matching regime as the sum of two contributions is the main result of this section. It remains to perform the explicit calculation of the integral \( C(\lambda, \zeta) \). This task can be accomplished by following the same procedure reported in [29]: the key point of this calculation amounts to finding the solution \( \beta^*(\zeta) \) of the saddle-point equation:

\[ \frac{\partial F(\lambda, \beta)}{\partial \beta} = 0. \]  

(46)

Details of the calculations are illustrated in Appendices VII A and VII B. Here we just provide the final result:

\[ \int_{\Gamma(\beta)}^{\beta} \frac{d\beta}{2\pi i} \frac{1}{\sqrt{N^{1/3} \beta}} e^{N^{1/3} F(\lambda, \beta)} \approx e^{-N^{1/3} \chi(\zeta)}, \]  

(47)

where the explicit form of \( \chi(\zeta) \) is discussed in Appendix VII C. Its asymptotic behaviours are:

\[ \chi(\zeta) = \begin{cases} \frac{3}{2} \left( \frac{\sigma}{\langle \epsilon \rangle} \right)^{2/3} & \zeta \to \zeta_l, \\ \sqrt{\frac{2}{\langle \epsilon \rangle}} \sqrt{-\frac{\sigma^2}{4\langle \epsilon \rangle} \zeta + O \left( \frac{1}{\langle \epsilon \rangle^3} \right)}, & \zeta \gg 1 \end{cases} \]  

(48)

where \( \zeta_l \) is the spinodal point for the localized phase, that is the smallest value of \( \zeta \) for which the saddle-point equation Eq. (46) admits a real solution, namely

\[ \zeta_l = \frac{3}{2} \left( \frac{\sigma^4}{\langle \epsilon \rangle} \right)^{1/3}. \]  

(49)

IV. THE FIRST-ORDER PHASE TRANSITION FROM A THERMALIZED PHASE TO LOCALIZATION

A. The microcanonical entropy in the matching regime

We are now in the position of retrieving the microcanonical partition function by computing the inverse Laplace transform of Eq. (10):

\[ \Omega_N(A, E) = \frac{1}{2\pi i} \int_{\lambda_0 - i\infty}^{\lambda_0 + i\infty} d\lambda \ e^{\lambda A} \tilde{\Omega}_N(\lambda, E) = e^{N \log(\pi)} \int_{\lambda_0 - i\infty}^{\lambda_0 + i\infty} d\lambda \ e^{N[a\lambda - \log(\lambda)]} \mathcal{Z}_N(\lambda, E), \]  

(50)

where the final expression on the r.h.s. of Eq. (50) stems from Eq. (13). In order to point out the presence of a phase transition we are interested to obtain an analytic estimate of \( \Omega_N(A, \zeta) \) in the matching regime, where \( \mathcal{Z}_N(\lambda, \zeta) \) is given by Eqs. (43) and Eq. (44) and \( \zeta = (E - E_{th})/N^{2/3} \approx O(1) \):

\[ \Omega_N(A, \zeta) = e^{N \log(\pi)} \int_{\lambda_0 - i\infty}^{\lambda_0 + i\infty} d\lambda \ e^{N[a\lambda - \log(\lambda)]} \left[ e^{-N^{1/3} \chi(\zeta)} + e^{-N^{1/3} \chi(\zeta)} \right]. \]  

(51)

In the thermodynamic limit, \( N \to \infty \), the leading contribution to the integral on the r.h.s. of Eq. (51) is given by the term \( N[a\lambda - \log(\lambda)] \), which determines the value of \( \lambda_0 \) as the solution of the saddle-point equation

\[ \frac{\partial}{\partial \lambda} [a\lambda - \log(\lambda)] = 0 \quad \Rightarrow \quad \lambda_0 = 1/a. \]  

(52)
The complete expression of $\Omega_N(A, \zeta)$ is thus obtained by replacing the multiplier $\lambda$ with its actual value $\lambda_0 = 1/a$. Accordingly, in the matching regime the complete partition function reads

$$\Omega_N(A, \zeta) \approx e^{N[1 + \log(\pi a)]} \left[ e^{-N^{1/3} \chi(\zeta)} + e^{-N^{1/3} \zeta^2/(2\sigma^2)} \right],$$

(53)

where $\sigma^2 = 20a^4$ and $\langle \varepsilon \rangle = 2a^2$, the latter expression being present in the definition of $\chi(\zeta)$ [see Eqns. (47), (48)]. This result provides us the expression for the microcanonical entropy at leading and sub-leading order in the thermodynamic limit:

$$S_N(A, \zeta) = N \left[ 1 + \log(\pi a) \right] - N^{1/3} \Psi(\zeta),$$

(54)

The leading term is extensive in $N$ and it represents a background entropy,

$$S_N^{\text{back}}(a) = N \left[ 1 + \log(\pi a) \right] = N s^{\text{back}}(a),$$

(55)

as the contribution of the bulk of the system at infinite temperature, which does not depend on $\zeta$, i.e. on the excess energy $\Delta E = E - E_{\text{th}}$, which is entirely adsorbed by the condensate. At sub-leading order the contribution to the microcanonical entropy in the thermodynamic limit is given by the function

$$\Psi(\zeta) = \inf_{\zeta} \left\{ \chi(\zeta), \zeta^2/(2\sigma^2) \right\},$$

(56)

and this allows us to identify the critical value $\zeta_c$ for localization as the one where the (subleading contribution to) entropy of the localized and that of the delocalized phase have identical magnitude, i.e., by the following matching condition

$$\chi(\zeta_c) = \zeta_c^2/(2\sigma^2).$$

(57)

The function $\Psi(\zeta)$ is shown in Fig. 3, more precisely, we have decided to draw it as a function of the rescaled variable $r = \zeta/\zeta_l$. From the argument discussed in App. VII D we find that the critical value of $r$, which does not depend on the parameters of individual energy distributions on lattice sites, is

$$r_c = \frac{\zeta_c}{\zeta_l} = 2^{1/3}.$$  

(58)

Since the derivative of $\Psi(\zeta)$ is discontinuous at $\zeta_c$, we can conclude that we are facing a first-order phase transition, from a thermalized phase to a localized one.
B. The order parameter: participation ratio

The first order transition can be further characterized by introducing the participation ratio of the energy per site

\[ Y_2 = \left( \frac{\sum_{j=1}^{N} \varepsilon_j^2}{N \sum_{j=1}^{N} \varepsilon_j} \right), \tag{59} \]

as a suitable order parameter, where the angular brackets denote the equilibrium average. From the definition in Eq. \(59\), we see that if the energy \( E \sim O(N) \) is distributed more or less democratically over all sites, then \( \varepsilon_j \sim O(1) \) for each \( j \). Hence, the numerator scales as \( N^2 \) and the denominator scales as \( N^2 \) and consequently \( Y_2 \sim 1/N \). In contrast, if an extensive amount of energy is localised at a single site (i.e., in the presence of a condensate), the numerator will scale as \( N^2 \) while the denominator still scales as \( N^2 \). Consequently, \( Y_2 \sim O(1) \) in the large \( N \) limit. Hence, the quantity \( Y_2 \) is a good measure to detect the localisation/condensation transition.

For our purposes it is enough to analyze the behavior of \( Y_2 \) in the proximity of the threshold energy, i.e., at \( E \sim E_{th} = N(\varepsilon) \) [see Sec. III.A], where, as discussed in the previous section, the transition point is located. In this regime the equilibrium joint probability distribution of local energies has, within the microcanonical ensemble, the following expression

\[ P(\varepsilon_1, \ldots, \varepsilon_N) = \frac{e^{N_s^{back}(a)}}{\Omega_N(A, E)} \prod_{j=1}^{N} f_a(\varepsilon_j) \delta \left( E - \sum_{j=1}^{N} \varepsilon_j \right), \tag{60} \]

where

\[ \Omega_N(A, E) = e^{N_s^{back}(a)} \int_0^\infty \prod_{j=1}^{N} [d\varepsilon_j f_a(\varepsilon_j)] \delta \left( E - \sum_{j=1}^{N} \varepsilon_j \right) \tag{61} \]

is the microcanonical partition function. In fact, as shown in the previous section [see the saddle-point condition in Eq. \(52\)], \( \Omega_N(A, E) \) in the matching regime can be written as a function of the probability distributions \( f_a(\varepsilon_j) \) of i.i.d. energy variables, where the label \( \lambda \) appearing in Eq. \(12\) can be replaced by the label \( a \), i.e. the inverse of the solution of the saddle-point condition. By plugging the expression of \( P(\varepsilon_1, \ldots, \varepsilon_N) \) written in Eq. \(60\) into the definition of \( Y_2 \) given in Eq. \(59\), we get:

\[ Y_2(E) = \frac{e^{N_s^{back}(a)}}{\Omega_N(A, E)} \int_0^\infty d\varepsilon d\varepsilon N \prod_{j=1}^{N} f_a(\varepsilon_j) \frac{\sum_{j=1}^{N} \varepsilon_j^2}{N \sum_{j=1}^{N} \varepsilon_j} \delta \left( E - \sum_{j=1}^{N} \varepsilon_j \right) \]

\[ = \frac{N e^{s^{back}(a)} E^2}{\Omega_N(A, E)} \int_0^\infty d\varepsilon \varepsilon^2 f_a(\varepsilon) \frac{\Omega_{N-1}(A, E - \varepsilon)}{\Omega_N(A, E)} \frac{\sum_{j=2}^{N} \varepsilon_j^2}{N \sum_{j=1}^{N} \varepsilon_j} \delta \left( E - \varepsilon - \sum_{j=2}^{N} \varepsilon_j \right) \]

\[ = \frac{N}{E^2} e^{s^{back}(a)} \langle \varepsilon^2 \rangle, \tag{62} \]

where it is important to recall that \( E^2 \sim N^2 \), so that

\[ Y_2(E) \sim \langle \varepsilon^2 \rangle / N. \tag{63} \]

In Eq. \(62\) we have then introduced the shorthand notation \( \rho(\varepsilon) \) for the marginal distribution of the energy \( \varepsilon \) on a single site, defined as

\[ \rho(\varepsilon) = f_a(\varepsilon) \frac{\Omega_{N-1}(A, E - \varepsilon)}{\Omega_N(A, E)}. \tag{64} \]

As a first step in the study of the behaviour of the order parameter \( Y_2 \) we observe that for \( E < E_{th} \) the marginal distribution \( \rho(\varepsilon) \) decays exponentially with \( \varepsilon \) on an energy scale which is independent of \( N \). The key point is the
calculation of $\Omega_{N-1}(A, E - \varepsilon)$, which, for very large values of $N$, can be approximated in a completely harmless way with $\Omega_N(A, E - \varepsilon)$. Since the value of the energy $\varepsilon$ on a single site can be at most $\varepsilon = E$, we have that the domain of the variable $y = E - \varepsilon$ is $y \in [0, E]$. Hence the integral which defines $\Omega_N(A, y = E - \varepsilon)$ through its inverse Laplace transform can be still computed by a saddle-point approximation:

$$\Omega_N(A, E - \varepsilon) = \int_{\beta_0 - i\infty}^{\beta_0 + i\infty} d\beta \exp \{ \beta(E - \varepsilon) + N \log[z(a, \beta)] \} \approx \exp \{ \beta_0(E - \varepsilon) + N \log[z(a, \beta_0)] \}$$

Accordingly, the participation ratio $Y_2$ vanishes as $1/N$ in the thermodynamic limit, i.e. in the thermalized phase close to $E_{th}$ localization of energy is, as expected, absent. For $E > E_{th}$ we cannot rely anymore on the saddle-point approximation for $\beta$ to compute the integral in Eq. (65). Still, from the study of $\Omega_N(A, E)$ we know that at the scale $E - E_{th} \sim N^{1/2}$ the partition function has a Gaussian shape. Therefore, we have that for values of $E$ up to the scale $E - E_{th} \sim N^{1/2}$ the marginal probability distribution of energy is given by the expression

$$\rho(\varepsilon) = f_a(\varepsilon) \exp[-(\Delta E - \varepsilon)^2/(2\sigma^2 N)] \quad \text{with} \quad \Delta E = E - E_{th},$$

By expanding the square in the numerator we obtain a term which simplifies with the denominator and we are left with the expression

$$\rho(\varepsilon) = f_a(\varepsilon) \exp \left[-\frac{\varepsilon^2}{2\sigma^2 N} + \frac{\varepsilon \Delta E}{\sigma^2 N} \right].$$

Recalling that $\Delta E \sim \sqrt{N}$, we can estimate the participation ratio by the relation

$$Y_2 \approx \frac{1}{N} \int_0^\infty d\varepsilon \varepsilon^2 f_a(\varepsilon) \exp \left[-\frac{\varepsilon^2}{2\sigma^2 N} + \frac{\varepsilon}{\sigma\sqrt{N}} \right].$$

In the limit of large $N$ this integral can be approximated as

$$Y_2 \approx \frac{1}{N} \int_0^\infty d\varepsilon \varepsilon^2 f_a(\varepsilon) \sim \frac{1}{N},$$

so that even for $E > E_{th}$ and $E - E_{th} \sim \sqrt{N}$ we have that the participation ratio vanishes asymptotically. The system is still in a delocalized phase, although the decay of $\rho(\varepsilon)$, as shown in Fig. 4, is not monotonic. With the same kind of argument it can be shown that even for $E - E_{th} \sim N^{2/3}$ the participation ratio vanishes asymptotically. The system is delocalized up to $E_c$, the critical value of the total energy (which is of order $O(N)$) where the first derivative of the entropy exhibits the discontinuity. Such a value $E_c$, according to Eq. (30), reads as:

$$E_c = E_{th} + N^{2/3}\zeta_c,$$

where $\zeta_c$ does not depend on $N$ and is determined by the matching condition in Eq. (57), see also Appendix VII D.

The situation is different for the case of extreme large deviations of the total energy, i.e., following the terminology of [29], for $E - E_{th} \sim N$. Also in this case the marginal distribution $\rho(\varepsilon)$ exhibits a bump (see Fig. 4). But in this case the whole $\rho(\varepsilon)$ is dominated in the large $N$ limit by the contribution of the bump, which, for fluctuations of order $\Delta E - \varepsilon \sim N^{1/2}$ around the bump center, reads as

$$\rho(\varepsilon) \approx \rho\text{bump}(\varepsilon) = f_a(\varepsilon) \frac{1}{N f(\Delta E)} \frac{1}{\sqrt{N}} \exp[-(\Delta E - \varepsilon)^2/(2\sigma^2 N)],$$

where we have used the fact that in the extreme large deviations regime the whole partition function is identical to $N$ times the distribution of the single variable (see [23, 26]), in formulae

$$\Omega_N(A, E) \approx N f_a(E - E_{th}).$$

Then, since we are interested to the estimate of $\rho\text{bump}(\varepsilon)$ for $\varepsilon \sim \Delta E$, we have that $f_a(\varepsilon)/f_a(\Delta E) = O(1)$ in the large $N$ limit, so that

$$\rho\text{bump}(\varepsilon) \approx \frac{1}{N^{3/2}} \exp[-(\Delta E - \varepsilon)^2/(2\sigma^2 N)] \approx \frac{1}{N} \delta(\Delta E - \varepsilon).$$
Since $\Delta E \sim N$, we finally obtain

$$\int_{0}^{\infty} d\varepsilon \varepsilon^2 \rho_{\text{bump}}(\varepsilon) = \frac{(\Delta E)^2}{N} \sim N,$$

so that

$$Y_2 = \frac{N}{E^2}(\varepsilon^2) \sim \text{const.}$$

The finite value of the participation ratio signals the localized phase. We want to point out that this scenario indicates that localization of energy is on a single site. In fact, the ratio between the width of the bump, of order $N^{1/2}$, and its position, $\Delta E \sim N$, vanishes asymptotically.

The overall situation can be summarized according to the following scheme, where the critical value of the energy $E_c$ is the one defined in Eq. (70) above:

(A) $E < E_{\text{th}}$: $\rho(\varepsilon)$ decays monotonically at large $\varepsilon$ and the participation ratio decays asymptotically as

$$Y_2(E) \sim \frac{1}{N}.$$  

(B) $E_{\text{th}} < E < E_c$: decay of $\rho(\varepsilon)$ at large values of $\varepsilon$ is non monotonic and the formation of a secondary bump can be easily seen in Fig. 4. This notwithstanding, the participation ratio still vanishes asymptotically as

$$Y_2(E) \sim \frac{1}{N};$$

we call this phase, which has been put in evidence also in another recent paper on constraint-driven condensation [30], the pseudo-condensate one.

(C) $E > E_c$: $\rho(\varepsilon)$ has a bump placed at $\varepsilon^* = (E - E_{\text{th}})$ and the participation ratio goes asymptotically to a constant value:

$$Y_2(E) \sim \text{const}.$$  

C. Negative temperatures

A straightforward consequence of the results reported in the previous subsections is that the only consistent definition of temperature for values of the energy density $e > e_{\text{th}} = E_{\text{th}}/N$ is the microcanonical one. Taking into account Gaussian fluctuations around $e_{\text{th}}$, i.e., $|e - e_{\text{th}}| \sim 1/N^{1/2}$, we have that the entropy density reads

$$s(a, e) = \lim_{N \to \infty} \frac{1}{N} \log[\Omega(a, e)] = -\frac{(e - e_{\text{th}})^2}{2\sigma^2}$$

so that the microcanonical temperature turns out to be:

$$\frac{1}{T} = \frac{\partial S_N(A, E)}{\partial E} = -\frac{1}{\sigma^2}(e - e_{\text{th}}).$$

The microcanonical temperature becomes negative as soon as the equivalence between ensembles is broken, that is, already for values of the specific energy above the threshold, i.e., $e > e_{\text{th}}$, but still lower than the critical value for localization, i.e., $e < e_c$. This means that for not too large values of $N$, which might be for instance the number of sites in a true optical lattice where an atomic condensate can be trapped, our analysis foresees the possibility to detect delocalized states with negative temperature. The fact that, above the threshold energy, temperature is negative irrespective of whether the asymptotic value of the order parameter is zero or not, reads off clearly from the expression of the microcanonical entropy in all the three regimes where $e > e_{\text{th}}$, 

$$S_N(A, E) = \begin{cases} \frac{N_s^{\text{back}} - N [e - e_{\text{th}}]^2 / (2\sigma^2)}{N} & e - e_{\text{th}} \sim N^{-1/2} \\ \frac{N_s^{\text{back}} - \Psi(\zeta)}{N} & e - e_{\text{th}} \sim N^{-1/3} \\ \frac{N_s^{\text{back}} - N^{1/2} \sqrt{e - e_{\text{th}}}}{N} & e - e_{\text{th}} \sim 1 \end{cases}$$
For instance, from Eq. \[81\] we have that the inverse temperature of the condensate reads

\[
\frac{1}{T} = \frac{\partial S_N(A,E)}{\partial E} = -\frac{1}{2N^{1/2}} \frac{1}{\sqrt{e - e_{th}}} \tag{82}
\]

Let us notice here that negative temperatures are not a peculiarity of the non-equivalence between canonical and microcanonical ensembles: they can be found and have a perfectly consistent physical meaning also in situations where the two ensembles are equivalent, provided that the Hamiltonian of the system is a bounded function \[31–33\]. On the other hand, in the case of unbounded Hamiltonian, e.g., the DNLSE studied here, negative temperatures have a physical meaning only within the microcanonical ensemble, thus making ensemble inequivalence a necessary condition for the observation of negative temperature states.

D. Finite-size effects and simulations: the pseudo-condensate phase

![Marginal energy density probability ρ(ε) obtained from numerical simulations for N = 128, a = 1 and different values of the energy density, namely ϵ = 2.00, 2.18, 2.35, 2.50, 2.70, 3.00, 3.41. The threshold energy (per d.o.f.) for the data in figure is e_{th} = 2 while the critical energy is e_{c} = 4.2.](image)

From the two previous section we have learned that there is an intermediate region of energies that we call the pseudo-condensate regime, \(e_{th} < \epsilon < e_{c}\), where a quite interesting phenomenon takes place: the order parameter decreases as \(1/N\) and the temperature is negative. Although in the thermodynamic limit \(N \to \infty\) this region vanishes [see Eq. \[86\] below] its existence is very important for numerical simulations and experiments, where the value of \(N\) is usually not too large. For instance, let us consider the case \(N = 128\) and \(a = 1\), that we have reproduced in numerical simulations. Since the Hamiltonian dynamics in the non-equivalence regime \(\epsilon > e_{th}\) suffers a critical slowing down, we have used the stochastic algorithm introduced in \[15\] and used also in \[26, 27\] for the investigation of constraint-driven condensation. In detail, we have considered random updates which guarantee the conservation of the two quantities:

\[
A = \sum_{j=1}^{N} \rho_{j}^{2} \quad E = \sum_{j=1}^{N} \rho_{j}^{4}. \tag{83}
\]

In particular, we have considered local random updates of triplets of neighbouring sites such that:

\[
\rho_{j-1}^{2}(t+1) + \rho_{j}^{2}(t+1) + \rho_{j+1}^{2}(t+1) = \rho_{j-1}^{2}(t) + \rho_{j}^{2}(t) + \rho_{j+1}^{2}(t)
\]

\[
\rho_{j-1}^{4}(t+1) + \rho_{j}^{4}(t+1) + \rho_{j+1}^{4}(t+1) = \rho_{j-1}^{4}(t) + \rho_{j}^{4}(t) + \rho_{j+1}^{4}(t), \tag{84}
\]

where the variable \(t\) is the discrete time of the algorithm and is measured in numbers of random moves divided by \(N\). After a transient of \(2^{16}\) time units, a stationary state is reached where we have sampled the marginal distribution \(\rho(\epsilon)\) for times up to \(t = 2^{27}\) units.
For $a = 1$ we have from the definitions in Eq. (17) that $\langle \varepsilon \rangle = 2$ and $\sigma^2 = 20$, respectively. This yields the following values for the spinodal point of the condensate and for the transition point in the scaling variable $\zeta$, which can be clearly seen in Fig. 3:

\[ \zeta_l \approx 8.77 \]
\[ \zeta_c \approx 11.05 \]  
(85)

The threshold energy $e_{th}$ for ensemble inequivalence and the localization energy $e_c$ reads off, accordingly, as:

\[ e_{th} = 2a^2 = 2 \]
\[ e_c = e_{th} + \frac{\zeta_c}{N^{1/3}} \approx 4.2 \]  
(86)

In terms of the order of magnitude of the typical energy per d.o.f., the extent of the pseudo-condensate regime can be thus fully appreciated at size $N = 128$. Fig. 4 shows that already at energies $e < e_c$, the bump of the condensate is clearly visible, although the system is in the pseudo-localized phase. Fig. 4 is indeed quite instructive: the non-monotonic decay of $\rho(\varepsilon)$ is not enough to say that the system is in the localized phase. In order to ascertain from data whether or not we are in the phase where the order parameter tends asymptotically to a finite value, a finite-size study of $\rho(\varepsilon)$ is necessary.

V. CONCLUSIONS AND PERSPECTIVES

In this manuscript we have shown how to compute the partition function of the Non-Linear Schrödinger Hamiltonian in Eq. (1) in the microcanonical ensemble and in the approximation of infinite temperature ($\beta = 0$). This has allowed us to present a clear and coherent scenario of the thermodynamics of this model, also in relation with its dynamical properties. In fact, previous approaches (e.g., see [7]) provided less transparent interpretations, due to the use of the grand-canonical ensemble for describing also the phase above the line $\beta = 0$ (see Fig.0). In fact, making use of the microcanonical approach we have been able to show that this is a condensate phase, where typically a finite fraction of the whole mass and energy are localized in a few lattice sites. According to Ruelle [34] this is exactly one of the two conditions where equivalence between statistical ensembles does not apply. Moreover, we have shown that the $\beta = 0$ line corresponds to a first-order phase transition from a thermalized phase to a localized one, characterized by a jump in the derivative $\partial S / \partial E$ of the microcanonical entropy with respect to the energy. In a dynamical perspective, this transition indicates the passage from a phase where equipartition holds to another phase where ergodicity is broken by the condensation mechanism.

There are further results emerging from our study, that merit to be mentioned. In the microcanonical ensemble the temperature can be computed by the formula $1/T = \partial S / \partial E$. We have shown that for $e < 2a^2$ the temperature is positive, then $T \to \infty$ when $e \to 2a^2$ and finally $T < 0$ when $e > 2a^2$. We want to point out that the change of sign of the temperature coincides with the formation of the condensate only in the thermodynamic limit. In fact, we have found that, for any finite value of the lattice size $N$, the true transition line for the condensate formation is slightly above the $\beta = 0$ line. Accordingly, for finite $N$ it exists a region where one can observe negative-temperature states, that are not yet localized. This is a particularly important outcome in the perspective of designing specific experiments of BEC in optical lattices, where such peculiar states can be observed, while avoiding the condensation of a large fraction of atoms onto a single or few sites.

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VII. APPENDICES

A. Derivation of the rate function \( \chi(\zeta) \) in the intermediate matching regime

In this Appendix we study the leading large \( N \) behavior of the integral in Eq. (44):

\[
\mathcal{C}(\lambda, \zeta) = N \int_{\Gamma(+)} \frac{d\beta}{i} \frac{1}{\sqrt{2\pi(\varepsilon)N^{1/3}}} e^{N^{2/3} F_\zeta(\beta)}
\]  

(87)

where \( \zeta \geq 0 \) can be thought of as a parameter and

\[
F_\zeta(\lambda, \beta) = \beta \zeta + \frac{1}{2} \sigma^2 \beta^2 + \frac{1}{2\beta}\epsilon \quad .
\]

(88)

It is important to recall that the contour \( \Gamma(+) \) is along a vertical axis in the complex \( \beta \)-plane with its real part negative, i.e. \( \text{Re}(\beta) < 0 \). Thus, we can deform this contour only in the upper left quadrant in the complex \( \beta \)-plane (\( \text{Re}(\beta) < 0 \) and \( \text{Im}(\beta) > 0 \)), but we cannot cross the branch cut on the real negative axis, nor can we cross to the \( \beta \)-plane where \( \text{Re}(\beta) > 0 \).

To evaluate the integral in Eq. (87), it is natural to look for a saddle point of the integrand in the complex \( \beta \) plane in the left upper quadrant, with fixed \( \zeta \). Hence, we look for solutions for the stationary points of the function \( F_\zeta(\lambda, \beta) \) in Eq. (88). They are given by the zeros of the cubic equation

\[
\frac{dF_\zeta(\beta)}{d\beta} = \zeta + \sigma^2 \beta - \frac{1}{2\beta}\epsilon = 0
\]

(89)

For brevity, making implicit the dependence on \( \lambda \) which appears just as fixed parameter, in what follows we will use the conventions below to denote partial derivatives with respect to \( \beta \):

\[
F'_\zeta(\beta) = \frac{\partial F_\zeta(\lambda, \beta)}{\partial \beta},
\]

\[
F''_\zeta(\beta) = \frac{\partial^2 F_\zeta(\lambda, \beta)}{\partial \beta^2}
\]

(90)

As \( \zeta \geq 0 \) varies, the three roots move in the complex \( \beta \) plane. It turns out that for \( \zeta < \zeta_1 \) (where \( \zeta_1 \) is to be determined), there is one positive real root and two complex conjugate roots. For example, when \( \zeta = 0 \), the three roots of Eq. (89) are respectively at \( \beta = (2\varepsilon\sigma^2)^{-1/2} \) with \( \phi = 0, \phi = 2\pi/3 \) and \( \phi = 4\pi/3 \). However, for \( \zeta > \zeta_1 \), all the three roots collapse on the real \( \beta \) axis, with \( \beta_1 < \beta_2 < \beta_3 \). The roots \( \beta_1 < 0 \) and \( \beta_2 < 0 \) are negative, while \( \beta_3 > 0 \) is positive. For example, in Fig. 4 we plot the function \( F'_\zeta(\beta) \) in Eq. (89) as a function of real \( \beta \), for \( \zeta = 12 \) and \( \lambda = 1 \) (so \( \sigma^2 = 20/\lambda^4 = 20 \)). One finds, using Mathematica, three roots at \( \beta_1 = -0.560164 \ldots \) (the lowest root on the negative side), \( \beta_2 = -0.170622 \ldots \) and \( \beta_3 = 0.130786 \ldots \). We can now determine \( \zeta_1 \) very easily. As \( \zeta \) decreases, the two negative roots \( \beta_1 \) and \( \beta_2 \) approach each other and become coincident at \( \zeta = \zeta_1 \) and for \( \zeta < \zeta_1 \), they split apart in the complex \( \beta \)-plane and become complex conjugate of each other, with their real parts identical and negative. When \( \beta_1 < \beta_2 \), the function \( F'_\zeta(\beta) \) has a maximum at \( \beta_m \) with \( \beta_1 < \beta_m < \beta_2 \) (see Fig. 4). As \( \zeta \) approaches \( \zeta_1 \), \( \beta_1 \) and \( \beta_2 \) approach each other, and consequently the maximum of \( F'_\zeta(\beta) \) between \( \beta_1 \) and \( \beta_2 \) approach the height 0. Now, the height of the maximum of \( F'_\zeta(\beta) \) between \( \beta_1 \) and \( \beta_2 \) can be easily evaluated. The maximum occurs at \( \beta = \beta_m \) where \( F''_\zeta(\beta) = 0 \), i.e., at \( \beta_m = -(\varepsilon\sigma^2)^{-1/3} \). Hence the height of the maximum is given by

\[
F'_\zeta(\beta = \beta_m) = \zeta + \sigma^2 \beta_m + \frac{1}{2\beta_m}\epsilon = \zeta - \frac{3}{2} \left( \frac{\sigma^4}{(\varepsilon)} \right)^{1/3}.
\]

(91)

Hence, the height of the maximum becomes exactly zero when

\[
\zeta = \zeta_1 = \frac{3}{2} \left( \frac{\sigma^4}{(\varepsilon)} \right)^{1/3}.
\]

(92)
FIG. 5. A plot of $F'_z(\beta) = \zeta + \sigma^2 \beta - \frac{1}{2}\langle \varepsilon \rangle \beta^2$ as a function of $\beta$ ($\beta$ real) for $\zeta = 12$, $\lambda = 1$ and $\sigma^2 = 20/\lambda^4 = 20$. There are three zeros on the real $\beta$ axis (obtained by Mathematica) at $\beta_1 \approx -0.56$, $\beta_2 \approx -0.17$ and $\beta_3 \approx 0.13$.

Thus we conclude that for $\zeta > \zeta_l$, with $\zeta_l$ given exactly in Eq. (92), the function $F'_z(\beta)$ has three real roots at $s = \beta_1 < 0$, $\beta_2 < 0$ and $\beta_3 > 0$, with $\beta_1$ being the smallest negative root on the real axis. For $\zeta < \zeta_l$, the pair of roots are complex (conjugates). However, it turns out (as will be shown below) that for our purpose, it is sufficient to consider evaluating the integral in Eq. (87) only in the range $\zeta > \zeta_l$ where the roots are real and evaluating the saddle point equations are considerably simpler. So, focusing on $\zeta > \zeta_l$, out of these 3 roots as possible saddle points of the integrand in Eq. (87), we have to discard $\beta_3 > 0$ since our saddle points have to belong to the upper left quadrant of the complex $\beta$ plane. Now, we deform our vertical contour $\Gamma_{(+)}$ by rotating it anticlockwise by $\pi/2$ so that it runs along the negative real axis. Between the two stationary points $\beta_1$ and $\beta_2$, it is easy to see [Fig. (5)] that $F''_z(\beta_1) > 0$ (indicating that it is a minimum along real $s$ axis) and $F''_z(\beta_2) < 0$ (indicating a local maximum). Since the integral along the deformed contour is dominated by the maximum along real negative $\beta$ for large $N$, we should choose $\beta_2$ to be the correct root, i.e., the largest among the negative roots of the cubic equation $\zeta + \sigma^2 \beta - 1/(2\langle \varepsilon \rangle \beta^2) = 0$. Thus, evaluating this saddle point (and discarding preexponential terms) we get for large $N$

$$C(\lambda, \zeta) \approx \exp[-N^{1/3}\chi(\zeta)]$$

(93)

where the rate function $\chi(\zeta)$ is given by

$$\chi(\zeta) = -F'_z(\beta = \beta_2) = -\beta_2 \zeta - \frac{1}{2}\sigma^2 \beta_2^2 - \frac{1}{2}\langle \varepsilon \rangle \beta_2^2$$

(94)

The right hand side can be further simplified by using the saddle point equation Eq. (89), i.e., $\zeta + \sigma^2 \beta_2 - 1/2\langle \varepsilon \rangle \beta_2^2 = 0$. We finally obtain

$$\chi(\zeta) = -\frac{\zeta \beta_2}{2} - \frac{3}{4\langle \varepsilon \rangle \beta_2}.$$  

(95)

B. Asymptotic behavior of $\chi(\zeta)$

We now determine the asymptotic behavior of the rate function $\chi(\zeta)$ in the range $\zeta_l < \zeta < \infty$, where $\zeta_l$ is given in Eq. (92). Essentially, we need to determine $\beta_2$ (the largest negative root) as a function of $\zeta$ by solving Eq. (89), and substitute it in Eq. (95) to determine $\chi(\zeta)$.

We first consider the limit $\zeta \to \zeta_l$ from above, where $\zeta_l$ is given in Eq. (92). As $\zeta \to \zeta_l$ from above, we have already mentioned that the two negative roots $\beta_1$ and $\beta_2$ approach each other. Finally at $\zeta = \zeta_l$, we have $\beta_1 = \beta_2 = \beta_m$.
where \( \beta_m = -\langle \varepsilon \rangle \sigma^2 \rangle^{-1/3} \) is the location of the maximum between \( \beta_1 \) and \( \beta_2 \). Hence as \( \zeta \to \zeta_i \) from above, \( \beta_2 \to \beta_m = -\langle \varepsilon \rangle \sigma^2 \rangle^{-1/3} \). Substituting this value of \( \beta_2 \) in Eq. (95) gives the limiting behavior

\[
\chi(\zeta) \to \frac{3}{2} \left( \frac{\sigma}{\langle \varepsilon \rangle} \right)^{2/3} \quad \text{as } \zeta \to \zeta_i
\]

(96)

as announced in the first line of Eq. (48).

To derive the large \( \zeta \to \infty \) behavior of \( \chi(\zeta) \) as announced in the second line of Eq. (48), it is first convenient to re-parametrize \( \beta_2 \) and define

\[
\beta_2 = -\frac{1}{\sqrt{2\langle \varepsilon \rangle \zeta}} \theta_\zeta.
\]

(97)

Substituting this in Eq. (89), it is easy to see that \( \theta_\zeta \) satisfies the cubic equation

\[
-b(\zeta) \theta_\zeta^3 + \theta_\zeta^2 - 1 = 0,
\]

(98)

where

\[
b(\zeta) = \sigma^2 \frac{1}{\sqrt{2\langle \varepsilon \rangle \zeta^{3/2}}}.
\]

(99)

Note that due to the change of sign in going from \( \beta_2 \) to \( \theta_\zeta \), we now need to determine the largest positive root of \( \theta_\zeta \) in Eq. (98). In terms of \( \theta_\zeta \), \( \chi(\zeta) \) in Eq. (95) reads

\[
\chi(\zeta) = \sqrt{\frac{2}{\langle \varepsilon \rangle}} \sqrt{\zeta - \frac{\sigma^2}{4\langle \varepsilon \rangle} \frac{1}{\zeta} + \mathcal{O} \left( \frac{1}{\zeta^{5/2}} \right)}.
\]

(100)

The representations in Eqs. (98), (99) and (100) are now particularly suited for the large \( \zeta \) analysis of \( \chi(\zeta) \). From Eq. (98), it follows that as \( \zeta \to \infty \), \( \theta_\zeta \to 1 \). Hence, for large \( \zeta \) or equivalently small \( b(\zeta) \), we can obtain a perturbative solution of Eq. (98). To leading order, it is easy to see that

\[
\theta_\zeta = 1 + \frac{b(\zeta)}{2} + \mathcal{O} \left( b(\zeta)^2 \right).
\]

(101)

with \( b(\zeta) \) given in Eq. (99). Substituting this in Eq. (100) gives the large \( \zeta \) behavior of \( \chi(\zeta) \)

\[
\chi(\zeta) = \sqrt{\frac{2}{\langle \varepsilon \rangle}} \sqrt{\zeta - \frac{\sigma^2}{4\langle \varepsilon \rangle} \frac{1}{\zeta} + \mathcal{O} \left( \frac{1}{\zeta^{5/2}} \right)}.
\]

(102)

as announced in the second line of Eq. (48).

C. Explicit expression of \( \chi(\zeta) \)

While the exercises in the previous subsections were instructive, it is also possible to obtain an explicit expression for \( \chi(\zeta) \) by solving the cubic equation Eq. (98) with Mathematica. The smallest positive root of Eq. (98), using Mathematica, reads

\[
\theta_\zeta = \frac{1}{3b_\zeta} + \frac{1}{3 \cdot 2^{2/3} b_\zeta} \left( 1 - i\sqrt{3} \right) \left( -2 + 27b_\zeta^2 + 3\sqrt{-12 + 81b_\zeta^2} \right)^{1/3} + \frac{1}{3 \cdot 2^{4/3} b_\zeta} \left( 1 + i\sqrt{3} \right) \left( -2 + 27b_\zeta^2 + 3\sqrt{-12 + 81b_\zeta^2} \right)^{1/3}
\]

(103)

where \( b_\zeta \), used as an abbreviation for \( b(\zeta) \), is given in Eq. (99). Using the expression of \( \zeta_i \) in Eq. (92), we can re-express \( b_\zeta \) conveniently in a dimensionless form

\[
b_\zeta^2 = \frac{1}{2} \left( \frac{2 \zeta_i}{3 \zeta} \right)^3.
\]

(104)
Consequently, the solution $\theta_\zeta$ in Eq. (103) in terms of the adimensional parameter $r = \zeta/\zeta_l \geq 1$ reads as

$$
\theta_\zeta \equiv \theta(r) = \frac{\sqrt{3}}{4} r^{3/2} \left[ 2 + \frac{(1 - i\sqrt{3})}{g(r)} + (1 + i\sqrt{3})g(r) \right]
$$

(105)

where

$$
g(r) = \frac{1}{r} \left( 1 + i \sqrt{r^3 - 1} \right)^{2/3}.
$$

(106)

By multiplying both numerator and denominator of $\theta(r)$ by $(1 - i \sqrt{r^3 - 1})^{2/3}$ one ends up, after a little algebra, with the following expression

$$
\theta(r) = \frac{\sqrt{3}}{4} r^{3/2} \left[ 2 + \frac{1}{r} \left( \xi u_r^{2/3} + \xi \pi_r^{2/3} \right) \right],
$$

(107)

where $\xi$ and $u_r$ denotes, respectively, a complex number and a complex function of the real variable $r$:

$$
\xi = 1 + i\sqrt{3},
\xi \equiv \frac{\sqrt{3}}{2} \rho \theta(r)
$$

(108)

and we have also introduced the related complex conjugated quantities:

$$
\xi = 1 - i\sqrt{3},
\pi_r = 1 - i \sqrt{r^3 - 1},
$$

(109)

We can then write the complex expressions in Eq. (107) both in their polar form, i.e., $u_r = \rho_r e^{i\phi_r}$ and $\xi = \rho e^{i\phi}$, with, respectively:

$$
\rho_r = r^{3/2},
\phi_r = \arctan(\sqrt{r^3 - 1})
$$

(110)

and

$$
\rho = 2,
\phi = \arctan(\sqrt{3}) = \frac{\pi}{3}.
$$

(111)

Finally, by writing $\xi$ and $u_r$ inside Eq. (107) in their polar form and taking advantage of the expressions in Eqns. (110), (111) we get:

$$
\theta(r) = \frac{\sqrt{3}}{4} r^{3/2} \left[ 2 + \frac{1}{r} \rho_r^{2/3} \left( e^{i(\phi + \frac{2}{3}\pi)} + e^{-i(\phi + \frac{2}{3}\pi)} \right) \right] = \\
= \frac{\sqrt{3}}{2} r^{3/2} \left[ 1 + 2 \cos \left( \frac{\pi}{3} + \frac{2}{3} \arctan(\sqrt{r^3 - 1}) \right) \right]
$$

(112)

In order to draw explicitly the function $\chi(\zeta)$, e.g. with the help of Mathematica, one can plug the expression of $\theta(r = \zeta/\zeta_l)$ from Eq. (112) into the following formula:

$$
\chi(\zeta) = \frac{\sqrt{\zeta}}{2\sqrt{2E}} \frac{\theta(\zeta/\zeta_l)^2 + 3}{\theta(\zeta/\zeta_l)},
$$

(113)

D. The critical value $\zeta_c$

We show here how to compute the critical value $\zeta_c$ at which $\chi(\zeta)$ equals $\zeta^2/(2\sigma^2)$, i.e., the value at which the two branches in Fig. 3 cross each other. To make the computations easier, it is convenient to work with dimensionless variables. Using $\zeta_l = (3/2)(\sigma^4/E)^{1/3}$ from Eq. (92), we express $\zeta$ in units of $\zeta_l$, i.e., we define

$$
r = \frac{\zeta}{\zeta_l} = \frac{2}{3} \left( \frac{E}{\sigma^4} \right)^{1/3}.
$$

(114)
In terms of $r$, one can rewrite $b(\zeta)$ in Eq. (99) as [using the shorthand notation $b_\zeta = b(\zeta)$]:

$$b_\zeta^2 = \frac{1}{2} \left( \frac{2}{3r} \right)^3.$$  \hfill (115)

Consequently, Eq. (98) reduces to

$$-\frac{1}{\sqrt{2}} \left( \frac{2}{3} \right)^{3/2} r^{-3/2} \theta(r)^3 + \theta(r)^2 - 1 = 0,$$

where $\theta(r) = \theta_{\zeta=r\zeta_l}$ is dimensionless. Quite remarkably, it turns out that to determine the critical value $\zeta_c$, rather conveniently we do not need to solve the above cubic equation, Eq. (116). Indeed, at $\zeta = \zeta_c$, i.e., $r = r_c$, equating $\chi(\zeta_c) = \zeta_c^2/2\sigma^2$, we get

$$\frac{\sqrt{\zeta_c}}{2\sqrt{2E}} \left[ \frac{\theta(r_c)^2 + 3}{\theta(r_c)} \right] = \frac{\zeta_c^2}{2\sigma^2}.$$  \hfill (117)

Expressing in terms of $r_c$, Eq. (117) simplifies to

$$\frac{\theta^2(r_c) + 3}{\theta(r_c)} = \frac{3^{3/2}}{2} r_c^{3/2}.$$  \hfill (118)

Consider now Eq. (116), evaluated at $r = r_c$. In this equation, we replace $r_c$ by its expression in Eq. (118). This immediately gives $\theta(r_c)^2 = 3/2$ and hence

$$\theta(r_c) = \sqrt{\frac{3}{2}}.$$  \hfill (119)

Using this exact $\theta(r_c)$ in Eq. (118) gives

$$r_c = \frac{\zeta_c}{\zeta_l} = 2^{1/3} = 1.25992\ldots$$  \hfill (120)

It is now straightforward to check that the expression of $\theta(r)$ written in Eq. (112) is consistent with the result just found, i.e., from it we retrieve $\theta(r_c) = 2^{1/3} = \sqrt{3/2}$. We have that

$$\theta(r_c) = 2^{1/3} = \frac{\sqrt{3}}{2} r_c^{3/2} \left[ 1 + 2 \cos \left( \frac{\pi}{3} + \frac{2}{3} \arctan(\sqrt{r_c^2 - 1}) \right) \right] =$$

$$= \sqrt{\frac{3}{2}} \left[ 1 + 2 \cos \left( \frac{\pi}{3} + \frac{2}{3} \arctan(1) \right) \right] = \sqrt{\frac{3}{2}} \left[ 1 + 2 \cos \left( \frac{\pi}{2} \right) \right] =$$

$$= \sqrt{\frac{3}{2}},$$

as expected.

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