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Phonon displacement distribution at $T = 0$

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Abstract

We compute the probability distribution function of the displacement squared of linearly coupled quantum oscillators in their ground state. We find it to be one of the extreme-value distributions, the Fisher–Tippett–Gumbel distribution, in $d = 1$, while it is a Gaussian in $d = 2, 3$ dimensions. We also discuss the crossover to non-Gaussian distributions (at $d = 2, 3$) at finite temperature T. We observe that the quantum effects remain important for sizes $\ell(T) \sim aT_D/T$, where a is the lattice spacing and T_D is the Debye temperature.

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1. Motivations

Distribution functions of global—i.e., space averaged—observables has proved a useful tool in characterizing and classifying a flurry of physical systems exhibiting complex behaviors characterized by scale invariant correlations. Applications range from turbulence and critical phenomena [1] to surface growth [2–5]. Indeed, it was only recently realized that such distribution functions fall in a limited number of universality classes according to a few ingredients like the symmetry properties of the underlying process from which they are built and space dimensionality. Here we present the first study of such a distribution function in a quantum system. We refer the reader to Ref. [6] for a recent review on the range of applications of those distribution functions.

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In the present paper, in contrast to existing studies, we focus on a quantum system in its ground state. Admittedly, we have chosen the simplest possible of all, namely linearly coupled oscillators. Nevertheless, we will show that even this textbook example hides rich and intriguing properties. The phonon spectrum displays $1/f$ type noise, as recently confirmed by Toshimitsu et al. [7], thus hinting at similar nontrivial distribution functions as already found in classical systems. This observation opens up the possibility to actually observe in a real system, if quantum, the connection between $1/f$ noise and the statistics of extremes amply explored e.g. in Ref. [3]. We shall also briefly describe the crossover from the ground-state properties to the finite-temperature behavior.

We start by defining our notations for the chain of quantum oscillators and then present the calculation of the distribution function of the space averaged displacement squared of those oscillators. Next we will state the results for higher dimensions (both of the embedding space and of the displacement vectors). Our closing discussion will be devoted to a short study of finite size and finite temperature effects in connection with possible experiments.

2. The quantum harmonic chain

2.1. Notations

For simplicity, we shall present the calculation for the case of the $d=1$ quantum harmonic oscillators. The quantity that we are interested in is the macroscopic mean-square displacement, w_2, in the position, u_j, of the atoms given by

$$w_2 = \sum_{j=1}^{N} u_j^2 \; . \tag{1}$$

In order to calculate it, we diagonalize the Hamiltonian of a linear chain of N coupled quantum harmonic oscillators

$$\hat{H} = \sum_{j=1}^{N} \left[\frac{1}{2}\,\pi_j^2 + \frac{1}{2}\,\omega_0^2 (u_{j+1} - u_j)^2 \right] \; , \tag{2}$$

where the mass of the particles is taken to be unity, π_j is the momentum conjugated to u_j, periodic boundary conditions are understood, and N odd is assumed for simplicity. The lattice spacing is denoted by a and the total length of the chain is $L = Na$. The Fourier transform of u_j is defined by

$$u_q = \frac{1}{N} \sum_j \mathrm{e}^{-\mathrm{i}qja} u_j, \quad q = \frac{2\pi n}{N}, \quad n = -(N-1)/2, \ldots, (N-1)/2 \; . \tag{3}$$

In terms of the Fourier modes, one has

$$\hat{H} = \sum_q \left[\frac{1}{2}\,\pi_q \pi_{-q} + \omega_q^2 u_q u_{-q} \right], \quad \omega_q = 2\omega_0 |\sin(qa/2)| \; . \tag{4}$$

Then defining the bosonic creation and annihilation operators

$$a_q = \frac{1}{\sqrt{2\hbar}}\left(\sqrt{\omega_q}u_q + \frac{\mathrm{i}}{\sqrt{\omega_q}}\pi_q\right), \quad a_q^\dagger = \frac{1}{\sqrt{2\hbar}}\left(\sqrt{\omega_q}u_{-q} - \frac{\mathrm{i}}{\sqrt{\omega_q}}\pi_{-q}\right), \tag{5}$$

we arrive at the textbook expression

$$\hat{H} = \sum_q \hbar\omega_q(a_q^\dagger a_q + \tfrac{1}{2}), \tag{6}$$

which we use as our starting point for the computation of the w_2 distribution function.

2.2. Generating function of the distribution

In order to find the distribution of w_2 one must evaluate

$$G(w_2) \equiv \left\langle \delta\left(w_2 - \frac{1}{N}\sum_j u_j^2\right)\right\rangle, \tag{7}$$

where the brackets $\langle\cdots\rangle$ denote a quantum and thermal average. It is convenient to pass to the Laplace transform

$$\tilde{G}(s) = \int_0^{+\infty} \mathrm{d}w_2\, G(w_2)\mathrm{e}^{-w_2 s} \tag{8}$$

and to substitute the Fourier modes

$$\tilde{G}(s) = \langle \mathrm{e}^{-(2s/N)\sum_{q>0} u_q u_{-q}}\rangle. \tag{9}$$

Making use of an integral representation we find

$$\hat{G}(s) = \prod_{q>0}\left[\int \frac{\mathrm{d}\bar{\psi}_q\,\mathrm{d}\psi_q}{2\pi}\,\mathrm{e}^{-\bar{\psi}_q\psi_q}\langle \mathrm{e}^{\mathrm{i}\sqrt{(2s/N)}\bar{\psi}_q u_q + \mathrm{i}\sqrt{(2s/N)}u_{-q}\psi_q}\rangle\right]. \tag{10}$$

Now we express u_q in terms of the creation and annihilation operators:

$$\begin{aligned}\left\langle \mathrm{e}^{\mathrm{i}\sqrt{(2s/N)}\bar{\psi}_q u_q + \mathrm{i}\sqrt{(2s/N)}u_{-q}\psi_q}\right\rangle = \mathrm{e}^{-(2s/N)(\hbar/2\omega_q)\bar{\psi}_q\psi_q}\\ \times\left\langle \mathrm{e}^{\mathrm{i}\sqrt{(2s/N)}\sqrt{(\hbar/2\omega_q)}(\psi_q a_{-q}^\dagger + \bar{\psi}_q a_q^\dagger)}\right.\\ \left.\times \mathrm{e}^{\mathrm{i}\sqrt{(2s/N)}\sqrt{(\hbar/2\omega_q)}(\psi_q a_q + \bar{\psi}_q a_{-q})}\right\rangle.\end{aligned} \tag{11}$$

At this stage several routes can be followed. We adopt the path-integral formulation for nonrelativistic quantum systems (as described in Ref. [8]) which requires to express the quantum observables in their normal ordered form before substituting the operators by their coherent state representation ($a_q \to \alpha_q,\ a_q^\dagger \to \bar{\alpha}_q$). To perform the latter step we have applied the formula $e^{A+B}=e^Ae^Be^{-\frac{1}{2}[A,B]}$ (valid if A and B commute with $[A,B]$). The expectation value to evaluate reads

$$\left\langle e^{(i\sqrt{2s}/N)\sqrt{(\hbar/2\omega_q)}\sum_{q>0}(\psi_q a^\dagger_{-q}+\bar{\psi}_q a^\dagger_q)}\ e^{(i\sqrt{2s}/N)\sqrt{(\hbar/2\omega_q)}\sum_{q>0}(\psi_q a_q+\bar{\psi}_q a_{-q})}\right\rangle$$
$$=\left\langle e^{i\sqrt{(2s/N)}\sqrt{(\hbar/2\omega_q)}\sum_q(\bar{h}_q\alpha_q(\beta)+\bar{\alpha}_q(\beta)h_q)}\right\rangle \tag{12}$$

with

$$h_q=\bar{\psi}_q,\quad \bar{h}_q=\psi_q \text{ for } q>0\,,$$
$$h_q=\psi_{-q},\quad \bar{h}_q=\bar{\psi}_{-q} \text{ for } q<0\,, \tag{13}$$

and the brackets in the r.h.s. of Eq. (12) denote the following path integral:

$$\int \mathscr{D}\bar{\alpha}\mathscr{D}\alpha\, e^{-S[\bar{\alpha},\alpha]+(i\sqrt{2s}/N)\sqrt{(\hbar/2\omega_q)}\sum_q(\bar{h}_q\alpha_q(\beta)+\bar{\alpha}_q(\beta)h_q)}=e^{-(2s/N)\sum_q \bar{h}_q\langle\bar{\alpha}_q\alpha_q\rangle h_q}\,, \tag{14}$$

where

$$S[\bar{\alpha},\alpha]=\sum_q\int_0^\beta d\tau\ \bar{\alpha}_q(\partial_\tau+\hbar\omega_q)\alpha_q \tag{15}$$

and the complex field α_q has the equal (Matsubara-)time correlator

$$\langle\bar{\alpha}_q\alpha_q\rangle=f_q\equiv\frac{1}{e^{\beta\hbar\omega_q}-1}\,. \tag{16}$$

Using Eqs. (10) and (12)

$$\tilde{G}(s)=\prod_{q>0}\left[\int\frac{d\bar{\psi}_q\,d\psi_q}{2\pi}\,e^{-\bar{\psi}_q\psi_q-(s/N)(\hbar/\omega_q)(1+f_q+f_{-q})\bar{\psi}_q\psi_q}\right] \tag{17}$$

leads to the final expression for the generating function

$$\hat{G}(s)=\prod_{q>0}\left[1+\frac{2s}{N}\frac{\hbar}{\omega_q}\left(\frac{1}{2}+f_q\right)\right]^{-1}\,. \tag{18}$$

In the ground-state all energy levels are empty, $f_q\overset{\beta\to\infty}{=}0$, hence

$$\hat{G}(s)=\prod_{q>0}\left[1+\frac{s}{N}\frac{\hbar}{\omega_q}\right]^{-1}\,. \tag{19}$$

We are now in a position to determine the first two moments of w_2:

$$\langle w_2\rangle=\frac{\hbar}{2\pi\omega_0}[\ln N+\gamma+\ln 2+\mathcal{O}(N^{-1})]\,,$$
$$\langle w_2^2\rangle-\langle w_2\rangle^2=\left(\frac{\hbar}{2\pi\omega_0}\right)^2\left[\frac{\pi^2}{6}+\mathcal{O}(N^{-1})\right]\,. \tag{20}$$

Note that $\langle w_2\rangle$ diverges logarithmically with N, a feature arising from the long-wavelength behavior of ω_q. In the limit $q \to 0$ the underlying lattice structure is not felt anymore and one is left with exactly the same quantities to compute as in Ref. [3]. In terms of the rescaled variable $x \equiv (w_2 - \langle w_2\rangle)/(\sqrt{\langle w_2^2\rangle - \langle w_2\rangle^2})$, the distribution function is denoted by $P(x)\,\mathrm{d}x = G(w_2)\,\mathrm{d}w_2$ with $P(x) = a\,\mathrm{e}^{-ax-\gamma-\mathrm{e}^{ax+\gamma}}$ ($a = \pi/\sqrt{6}$, γ is the Euler constant) being the celebrated extreme-value statistics Fisher–Tippett–Gumbel (FTG) distribution. In order to illustrate the speed of convergence of P towards its FTP limiting form, we have numerically evaluated it for a finite 21 site lattice, with the result, shown in Fig. 1, that it cannot be distinguished from its $N = \infty$ form.

At high temperature we approximate

$$f_q \overset{\beta\to 0}{\simeq} \frac{1}{\beta\omega_q} \tag{21}$$

hence

$$\hat{G}(s) \simeq \prod_{q>0}\left[1 + \frac{2s}{N}\frac{\hbar}{\beta\omega_q^2}\right]^{-1}, \tag{22}$$

which results [3] in $P(x)$ being the ϑ_4 Jacobi function. In higher space dimensions $d > 1$ the formula yielding the generating function for the distribution of $(1/N)\sum_{\mathbf{r}} \mathbf{u}_{\mathbf{r}}^2$

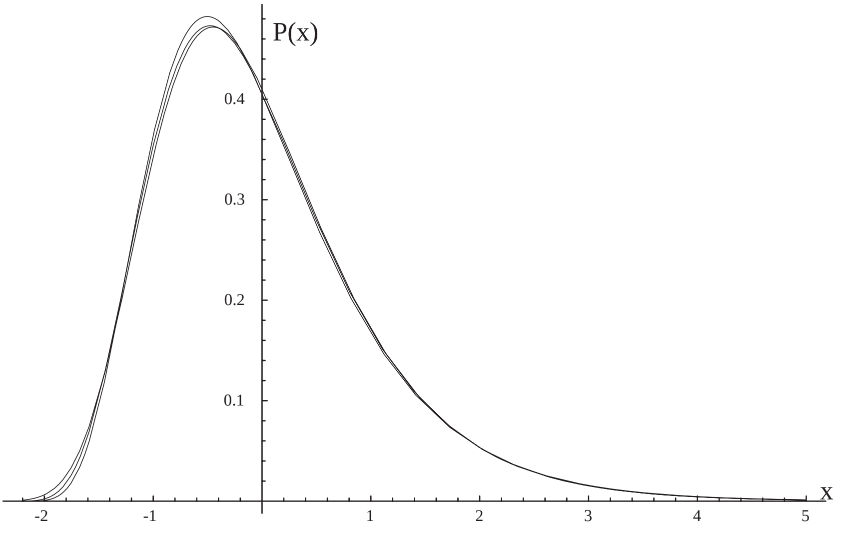

Fig. 1. We have superimposed the plots of the rescaled distribution function $P(x)$ as a function of $x \equiv (w_2 - \langle w_2\rangle)/\left(\sqrt{\langle w_2^2\rangle - \langle w_2\rangle^2}\right)$ for $N = 21$ lattice sites with both the exact FTG distribution and the continuum limit analog of P given in Ref. [3] (in which $\omega_q = \omega_0 qa$ for all q).

(with $\mathbf{u_r}$ the local displacement of the atom located at site $\mathbf{r}$) in the ground state can be easily found to be

$$\hat{G}(s) = \prod_{\mathbf{q},\varepsilon} \left[1 + \frac{2s}{N} \frac{\hbar}{\omega_{\mathbf{q},\varepsilon}} \left(\frac{1}{2} + f_{\mathbf{q},\varepsilon} \right) \right]^{-1} , \tag{23}$$

where the product extends over half the Brillouin zone and over the polarization directions ε and where $\omega_{\mathbf{q},\varepsilon}$ is the frequency of mode $\mathbf{q}$ in polarization state ε. For an isotropic hypercubic lattice one has $\omega_{\mathbf{q}}^2 = 2\omega_0 \sum_{\mu=1}^{d} (1 - \cos(q_\mu a))$, independently of the d polarization directions. Note that a similar formula could be easily derived for other geometries of experimental relevance (such as a tube). The mathematics for $d > 1$ is similar to that performed by Bramwell et al. [9] and we shall not reproduce it here. We deduce that in space dimension $d = 2, 3$ the distribution function is Gaussian, but crosses over to nontrivial shapes at finite temperature. This originates from the fact that the momentum integral entering the expression of the variance diverges at large wavelengths. As can be seen by balancing the ground-state contribution and the finite-temperature ones, small systems of linear size L such that

$$f_q \simeq \mathcal{O}(1) \quad \text{for } q = \mathcal{O}(L^{-1}) , \tag{24}$$

that is for system sizes such that $L \lesssim \ell(T) = aT_D/T$, where a is the lattice spacing and T_D is the Debye temperature, ground-state properties will dominate.

3. Final comments

Several comments are in order. In real one-dimensional systems the atoms are pinned to their equilibrium position by a local confining potential. In principle this modifies the dispersion relation and introduces a low momentum cut-off that will potentially destroy the FTG form of G. If the pinning energy is not too strong with respect to the Debye temperature, one should at least observe strong deviations from a Gaussian distribution, if not the full FTG function.

An important experimental and theoretical issue is that of resistivity fluctuations in the ground state. Our computation indicates that vacuum fluctuations alone could lead to nontrivial behaviors, even if we are aware that far more important physical effects will come into play (impurities). Indeed, any measurement of the chain properties will necessarily involve excitations (e.g. through the scattering of electrons) and provide information departing from ground state properties [10]. Nevertheless, returning to the explicit formulas, one sees that the crossover between quantum and classical behaviour will be observable at sizes of the order of $\ell_{\text{cross}} = a(\hbar\omega_0/k_B T) \sim a(T_D/T)$, where T_D is the Debye temperature. Hence the FTG distribution function should survive at finite (but small) temperatures for mesoscopic systems.

As a final remark we emphasize the extremely intriguing connection between the extreme value statistics and the ground state of one-dimensional phonons. We have been unable to come by any qualitative explanation of this mathematical, yet intuition-challenging, observation.

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